TaPS: A Performance Evaluation Suite for Task-based Execution Frameworks

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Enabling eScience Applications

Better Benchmarking

TaPS: Task Performance Suite

~~Evaluation~~ *Exploration*

Let's Put the Science in eScience

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***Abstract*—The underlying premise behind eScience is that computational methods and data-driven approaches can contribute to scientific discovery on a par with, or even superior to, traditional experimental methods; that the combination of computers, software, and extant data collections are the modern equivalent to the scientific instruments that have led to our understanding of fundamental laws in physics, chemistry, biology, and other domains. However, a robust methodology for making the results of eScience activities "scientific" is lacking, with significant consequences. In this brief paper we propose a shift in perspective as to what it means to create an eScience-based result and how the scientific validity of eScience experiments might be improved.**

***Index Terms*—escience, scientific method, reproducablity, d… management**

II. A Change of Perspective

Errors such as those described above persist in spite of the use of widely accepted tools such as shared storage systems, workflow management tools, and software and data repositories. We argue here that these persistent problems are a consequence not of inherent deficiencies in the tools used, but of methodologies that are overly focused on documenting the process that was followed to produce published results (e.g., software stack, the sequence of computational steps taken,

"The underlying premise behind **eScience** is that **computational methods** and **data-driven approaches** can contribute to scientific discovery on a par with, or even superior to, traditional experimental methods"

eScience *Paradigms* (non-exhaustive)

Machine Learning

Text Summarization towards Scientific Information Extraction

Asynchronous Decentralized Bayesian Optimization for Large Scale Hyperparameter Optimization

FLoX: Federated Learning with FaaS at the Edge

Nikita Kotsehub*, Matt Baughman†, Ryan Chard‡, Nathaniel Hudson†‡, Panos Patros§, Omer Rana¶, Ian Foster†‡, Kyle Chard†‡

Distributed/High-Perf. Computing

Lazy Python Dependency Management in Large-scale systems

PSI/J: A Portable Interface for Submitting, Monitoring, and Managing Jobs

Federated Function as a Service for eScience

Yadu Babuji*, Josh Bryan*, Ryan Chard*, Kyle Chard*, Ian Foster*, Ben Galewsky+, Daniel S. Katz+, Zhuozhao Li*

*University of Chicago, +University of Illinois at Urbana-Champaign

Data-Driven/Provenance

Database Evolution, by Scientists, for Scientists: A Case Study

A Method for Constructing Research Data Provenance in High-Performance Computing Systems

Can Automated Metadata Extraction make Scientific Data More Navigable?

Tyler J. Skluzacek, Kyle Chard, Ian Foster

Computational Workflows

Extreme Scale Survey Simulation with Python Workflows

Running Ensemble Workflows at Extreme Scale: Lessons Learned and Path Forward

WfChef: Automated Generation of Accurate Scientific Workflow Generators

Towards Lightweight Data Integration using Multi-workflow Provenance and Data Observability

Renan Souza, Tyler J. Skluzacek, Sean R. Wilkinson, Maxim Ziatdinov, Rafael Ferreira da Silva

Papers featured in eScience 2021—2023

Modern eScience Applications are *Task-centric*

Applications are composed as a set of **discrete tasks** designed to **automate** computational processes to achieve a **scientific goal**

Benefits

- Heterogeneous Resources
- Software Modularity
- Monitoring
- Performance
- Reproducibility
- *and many more!*

Applications [1]

- Bioinformatics
- Cosmology
- High Energy Physics
- Materials Science
- Molecular Dynamics
- *and many more!*

Challenges [2]

- Coupling AI/ML/Quantum
- Cloud and HPC Integration
- Data Flow/Provenance
- Standards/Interoperability
- Performance
- *and many more!*

[1] "Scientific Workflows: Moving Across Paradigms" (https://dl.acm.org/doi/10.1145/3012429)
[2] Workflows Community Summit (https://arxiv.org/abs/2304.00019)

How do we build and execute task-based eScience applications?

Task Execution Frameworks

Manage the execution of tasks in parallel across arbitrary hardware.

Task Execution Frameworks

Workflow Management Systems

Define, manage, and execute workflows represented by a directed acyclic graph (DAG) of tasks

Explicit

DAG defined via configuration file or domain specific language

Apache Airflow
FireWorks
nextflow
Pegasus
swift

Implicit

Task dependencies derived through dynamic evaluation of a procedural script

dask
Parsl
TaskVine
RAY

Concurrent Executors

On-demand asynchronous execution of tasks

AWS Lambda

- Enabling eScience Applications
- **Better Benchmarking**
- TaPS: Task Performance Suite
- ~~Evaluation~~ *Exploration*

The Status Quo

Ad Hoc Benchmarks

- Extensions of framework-specific examples or demos
- One-off/custom evaluation scripts for a publication
- Forks of real science applications

Problems

- Code is **framework-specific**
- Ad-hoc scripts subject to **code rot**
- Porting applications can be **onerous**
- Subtle **errors** in ported applications can lead to **inaccurate comparisons**

SimGrid: a Generic
Large-Scale Distribut
Univer

Developing accurate and scalable simu
management systems with WRENCH

Application skeletons: Construction and use in
Daniel S. Katz[a,*], Andre Merzky[b], Zhao Zhang[c], Shantenu Jha[b]
[a] Computation Institute, University of Chicago & Argonne National Laboratory, Chicago, IL, USA
[b] RADICAL Laboratory, Rutgers
[c] AMPLab, University of Califo

WfCommons: A Framework for Enabling Scientific Workflow Research and Development
Tainã Coleman[a,c,*], Henri Casanova[b], Loïc Pottier[a], Manav Kaushik[c], Ewa Deelman[a,c], Rafael Ferreira da Silva[a,c,*]

WfBench: Automated Generation of Scientific Workflow Benchmarks
Tainã Coleman*, Henri Casanova† Ketan Maheshwari‡, Loïc Pottier*, Sean R. Wilkinson‡
Justin Wozniak§, Frédéric Suter‡, Mallikarjun Shankar‡, Rafael Ferreira da Silva‡
niversity of Hawaii, Honolulu, HI, USA
onal Laboratory, Oak Ridge, TN, USA

Prior work focused on **simulations** and **synthetic workloads**

We lack a **standardized** set of real applications/workloads for benchmarking task executors.

Drawing Inspiration from Other Fields

Systems

The **LINPACK Benchmarks** are a measure of a system's floating-point computing power. Introduced by Jack Dongarra, they measure how fast a computer solves a dense *n* by *n* system of linear equations *Ax* = *b*, which is a common task in engineering.

TOP 500 The List.

TPC Transaction Processing Performance Council

byte-unixbench

UnixBench is the original BYTE UNIX benchmark suite, updated and revised by many people over the years.

AI/ML

ML Commons

MLPerf

Papers With Code

FaaS

FunctionBench

FAASDOM: A Benchmark Suite for Serverless Computing

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SeBS: The Serverless Benchmark Suite

Evaluate supported serverless platforms with real-world benchmarks.

Performance & Cost
Invocation Overhead
Container Eviction
Serverless Communication*
Serverless Workflows*
GPU Functions*

APACHE OpenWhisk

python

node JS

*Experimental and work-in-progress features.

Goals of a Good Benchmark

- Objective metrics
- Facilitate meaningful comparison
- Transparency and reproducibility
- Common ground
- Democratize research
- Accelerate advancements

Enabling eScience Applications

Better Benchmarking

TaPS: Task Performance Suite

~~Evaluation~~ *Exploration*

TaPS: Task Performance Suite

A standardized framework for evaluating task execution frameworks with real and synthetic science applications

TaPS: Task Performance Suite

- Audience
- Architecture
- Applications
- Framework
- Plugin System
- Using TaPS

Audience

Systems Software Developers & Application Builders

Anyone with questions like:

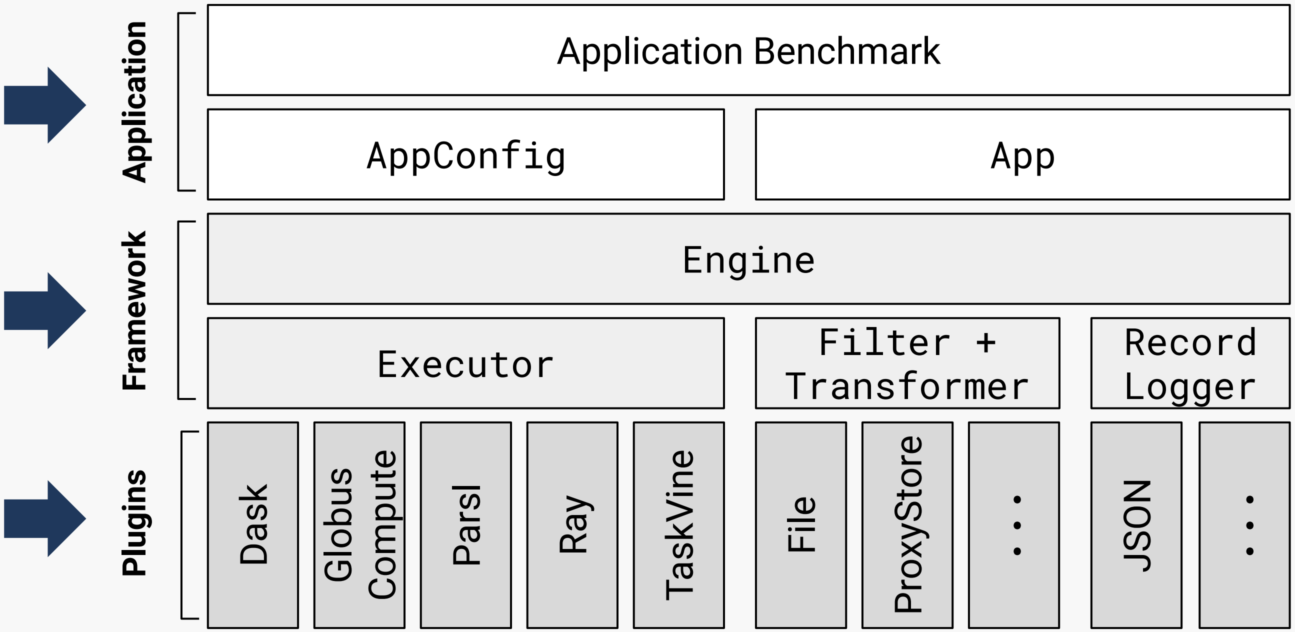
- ➔ How do I evaluate my:
  - ◆ distributed execution framework?
  - ◆ data management system?
  - ◆ modifications to existing systems?
- ➔ What are the performance characteristics of prior work?
- ➔ Which task executor performs best for similar workloads to mine?

Architecture

Use reference Apps or add your own

Engine: Glue that integrate Apps with Engine Plugins

Use provided Engine Plugins or your own

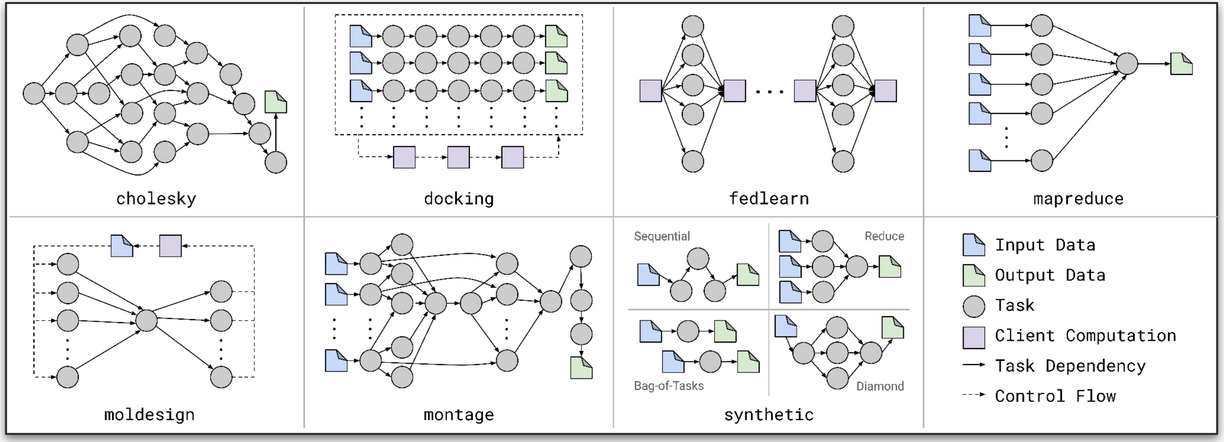


https://taps.proxystore.dev/latest/api/

Applications

- ➔ Six Real Apps
- ➔ Two Synthetic
- ➔ Diverse Patterns
- ➔ Diverse Domains
- ➔ Configurable
- ➔ Per-App Guides

Type	Name	Domain	Task Type(s)	Data Type(s)
Real	**cholesky**	Linear Algebra	Python	In-memory
	docking	Drug Discovery	Executable, Python	File
	fedlearn	Machine Learning	Python	In-memory
	mapreduce	Text Analysis	Python	File, In-memory
	moldesign	Molecular Design	Python	In-memory
	montage	Astronomy	Executable	File
Synthetic	**synthetic**	—	Python	In-memory
	failures	—	*Depends on base app*	*Depends on base app*



https://taps.proxystore.dev/latest/apps/

How to design an interface **expressive** enough to build these applications but simple enough to **unify** task executors?

Task Execution Frameworks

Workflow Management Systems

Define, manage, and execute workflows represented by a directed acyclic graph (DAG) of tasks

Explicit ✗

DAG defined via configuration file or domain specific language

Implicit ✓

Task dependencies derived through dynamic evaluation of a procedural script

Concurrent Executors ✓

On-demand asynchronous execution of pure tasks

Why are explicit WMSs not Supported?

- Static DAGs not expressive enough for dynamic/procedural applications
- DSLs are tightly coupled/unique to WMS
- *Possible* but requires complex per-DSL parsing and code generation

Engine

Interface between Apps and Plugins

- ➔ Apps submit tasks to Engine and gets back a `TaskFuture`
- ➔ `TaskFuture` can be an argument for other tasks (implicit data flow dependency)
- ➔ `Engine` invokes plugins (e.g., submit task to `Executor`)

Protocol: concurrent.futures `Executor`

- ➔ Closest to "standard" in Python ecosystem
- ➔ Easy to port existing apps using an `Executor`
- ➔ Protocol extended to require implicit data flow dependencies via futures

```python
class Engine:
    def __init__(
        self,
        executor: Executor,
        filter: Filter | None = None,
        transformer: Transformer | None = None,
        logger: RecordLogger | None = None,
    ) -> None: ...

    def submit(
        self,
        function: Callable[P, T],
        *args: P.args,
        **kwargs: P.kwargs,
    ) -> TaskFuture[T]: ...

    def map(
        self,
        function: Callable[P, T],
        *iterables: Iterable[P.args],
        ...
    ) -> Iterator[T]: ...

    def shutdown(self, ...) -> None: ...

def as_completed(...) -> Generator[TaskFuture[T]]: ...

def wait(...) -> tuple[DoneTasks, NotDoneTasks]: ...
```

Plugins

Used by Apps

Engine Plugins — Task Execution

Interface: Executor*

```
class Executor:
    def submit(
        self,
        function: Callable[P, T],
        *args: P.args,
        **kwargs: P.kwargs,
    ) -> Future[T]: ...

    def map(
        self,
        function: Callable[P, T],
        *iterables: Iterable[P.args],
        ...
    ) -> Iterator[T]: ...

    def shutdown(self, ...) -> None: ...
```

*Requires support for implicit data via futures. Wrapper provided for implementations that lack this feature.

Purpose: Asynchronously execute functions

Implementations:

- ThreadPool
- ProcessPool
- Dask
- Globus Compute
- Parsl
- Ray
- TaskVine

Future Extensions:

- Cloud FaaS
- New Executors

Engine Plugins — Data Management

Interface: `Filter` and `Transformer`

```
class Filter:
    def __call__(self, obj: Any) -> bool:
        ...

class Transformer(Generic[IdentifierT]):
    def is_identifier(self, obj: T) -> bool:
        ...

    def transform(self, obj: T) -> IdentifierT:
        ...

    def resolve(self, id_: IdentifierT) -> Any:
        ...
```

Purpose: Manage task data by filtering and transforming data into/resolve data from intermediate representations

Implementations:

- Shared File Systems
- ProxyStore (DAOS, Globus Transfer, Margo, Redis, UCX, ZMQ, …)

Future Extensions:

- Cloud Storage

Engine Plugins — Task Logging

Interface: `RecordLogger`

```
Record: TypeAlias = Dict[str, Any]

class RecordLogger:
    def log(self, record: Record) -> None:
        ...
```

Purpose: Record task execution traces

Implementations:

- JSON

Future Extensions:

- Databases
- WfTrace format

Adding an Engine Plugin

- ➔ Config types for each plugin
- ➔ Contains all user-controllable parameters (optional defaults)
- ➔ `@register(<type>)` decorator
  - Registers plugin type with TaPS
  - Plugin name and parameters exposed in CLI choices / config file parser
  - Parameter validation auto-generated from fields
- ➔ `get_<type>()` used by TaPS

```python
import globus_compute_sdk
from concurrent.futures import Executor
from pydantic import Field
from taps.executor import ExecutorConfig
from taps.executor.utils import FutureDependencyExecutor
from taps.plugins import register

@register('executor')
class GlobusComputeConfig(ExecutorConfig):
    """Globus Compute Executor plugin configuration."""

    name: Literal['globus'] = Field('globus', description='Name.')
    endpoint: str = Field(description='Endpoint UUID.')
    batch_size: int = Field(128, description='Batch size.')

    def get_executor(self) -> Executor:
        """Initialize an executor from the config."""
        executor = globus_compute_sdk.Executor(
            self.endpoint,
            batch_size=self.batch_size,
        )
        return FutureDependencyExecutor(executor)
```

Utility for adding implicit data flow support to any executor

https://taps.proxystore.dev/latest/guides/executor/

Adding an Application

Config

```python
from typing import Literal
from pydantic import Field
from taps.apps import App, AppConfig
from taps.plugins import register

@register('app')
class CholeskyConfig(AppConfig):
    """Cholesky application configuration."""

    name: Literal['cholesky'] = Field('cholesky', ...)
    matrix_size: int = Field(description='Matrix size.')
    block_size: int = Field(description=Block/tile size.')

    def get_app(self) -> App:
        """Create an application instance from the config."""
        from taps.apps.cholesky import CholeskyApp

        return CholeskyApp(
            matrix_size=self.matrix_size,
            block_size=self.block_size,
        )
```

App

```python
import pathlib
from taps.engine import Engine

class CholeskyApp:
    """Cholesky decomposition application."""

    def __init__(self, matrix_size: int, block_size: int) -> None:
        self.matrix_size = matrix_size
        self.block_size = block_size

    def close(self) -> None:
        """Clean up and close the application."""
        pass

    def run(self, engine: Engine, run_dir: pathlib.Path) -> None:
        """Run the application."""
        future = engine.submit(func, *args, **kwargs)
        future.result()
```

Application logic goes inside `run()` and interfaces with `Engine`

https://taps.proxystore.dev/latest/guides/apps/

Using TaPS

Execute benchmarks with CLI or programmatically via API

```
$ python -m taps.run \
    --app cholesky --app.matrix-size 10000 --app.block-size 1000 \
    --engine.executor dask --engine.executor.workers 16 \
    --engine.transformer proxystore {transformer options} \
    --engine.filter object-size {filter options} \
    ...

[Output Truncated]
RUN   (taps.run) :: Runtime directory: runs/cholesky-dask-2024-09-19-12-00-00
APP   (taps.apps.cholesky) :: Generated input matrix: (10000, 10000)
APP   (taps.apps.cholesky) :: Block size: 1000
APP   (taps.apps.cholesky) :: Output matrix: (10000, 10000)
RUN   (taps.run) :: Finished app (name=cholesky, runtime=13.18s)
```

Run directory:

- ➔ Logs for analysis
- ➔ Config for reproducibility
- ➔ Application outputs

```
+ runs
  ├ cholesky-dask-2024-09-19-11-00-00
  └ cholesky-dask-2024-09-19-12-00-00
     ├ config.toml
     ├ log.txt
     └ tasks.jsonl
```

```
[app]
name = "cholesky"
matrix_size = 10000
block_size = 1000

[engine.executor]
name = "dask"
workers = 16

[engine.filter]
name = "object-size"
min_size: 1000

[engine.transformer]
name = "proxystore"
cache_size = 16
extract_target = true
populate_target = true
...

[logging]
level = "INFO"
file_level = "INFO"
file_name = "log.txt"

[run]
dir_format = "runs/{name}-{executor}-{timestamp}"
```

https://taps.proxystore.dev/latest/guides/config/

```
python -m taps.run --config config.toml
```

- **Enabling eScience Applications**
- **Better Benchmarking**
- **TaPS: Task Performance Suite**
- **~~Evaluation~~ *Exploration***

~~Evaluation~~ *Exploration* Goals

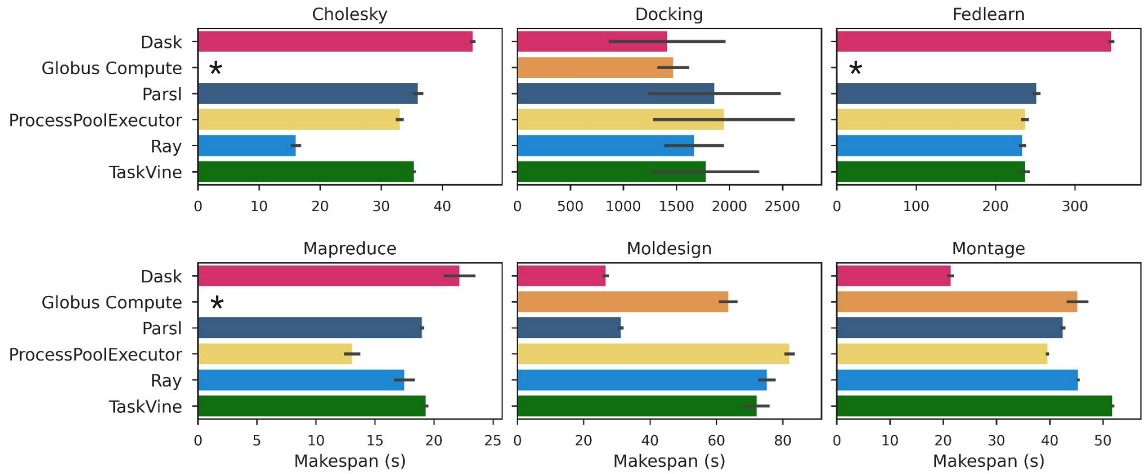
- ✗ *Not* to determine which executor is best
- ✓ Showcase kinds of evaluations TaPS can support
- ✓ Showcase characteristics of applications and executors
- ✓ Leave with more questions than answers… keep exploring!
- ✓ Encourage more discourse on benchmarking in the community

https://github.com/proxystore/escience24-taps-analysis

Application Makespan

No stand-out executor; new questions to pose.

- ➔ Why are some combos so much faster? (Ray in Cholesky, Dask/Parsl in Moldesign, and Dask in Montage)
- ➔ Which benefit more from warm-starts?
- ➔ How does performance correlate to average task duration or data flow volume?
- ➔ How do they handle resource contention with nested parallelism (e.g., OpenMP tasks)



Application	Workers	Task Count	Max Serialized Object Size	Parameters
cholesky	64	385	24 MB	Matrix Size: 10 000×10 000, Block Size: 1000×1000
docking	32	192	$O(1)$ kB	Initial Simulations: 3, Batch Size: 8, Rounds: 3
fedlearn	32	48	20 MB	Dataset: MNIST, Clients: 16, Batch Size: 32, Rounds: 3, Epochs/Round: 1
mapreduce	32	33	114 MB	Dataset: Enron Email Corpus, Map Task Count: 32
moldesign	32	346	$O(1)$ MB	Initial Simulations: 16, Batch Size: 16, Search Count: 64
montage	32	419	$O(1)$ kB	—

https://github.com/proxystore/escience24-taps-analysis

*Task data exceeds Globus Compute 10 MB payload limit.

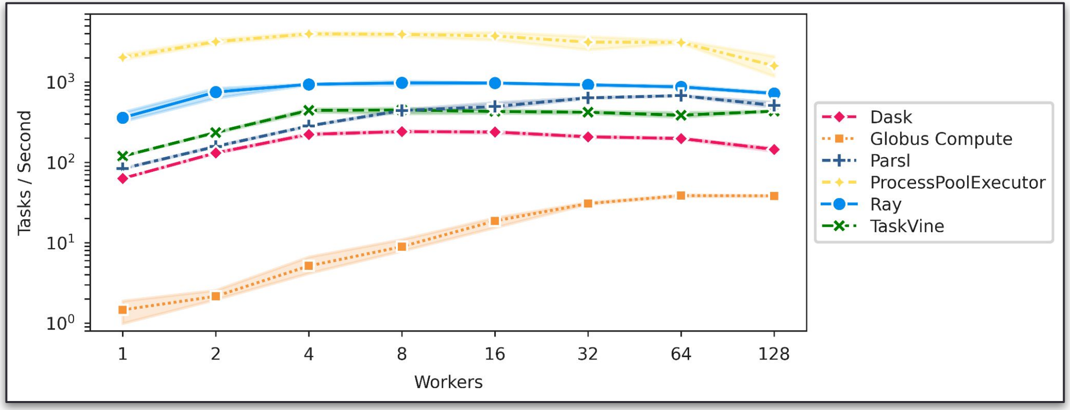
Scheduler Performance – Scaling Workers

Workload

- Synthetic App – Bag of Tasks
- Vary *n* workers. Submit *n* initial tasks
- Submit tasks as prior complete
- Record task throughput

Hardware

- Single CHI@TACC compute-zen-3 node
- 2x AMD EPYC 7763 64-Core CPU
- 256 Logical Cores / 256 GB RAM



➔ **ProcessPool** (yellow) is high-water mark (no scheduler)
➔ **Ray** (light blue) has lowest task latency but does not scale well
➔ **Dask** (pink) and **TaskVine** (green) plateau between 4–8 workers
➔ **Parsl** (dark blue) scales best but has higher individual task latency
➔ **Globus Compute** (orange) does better when batching more tasks

https://github.com/proxystore/escience24-taps-analysis

Scheduler Performance – Data Transfer

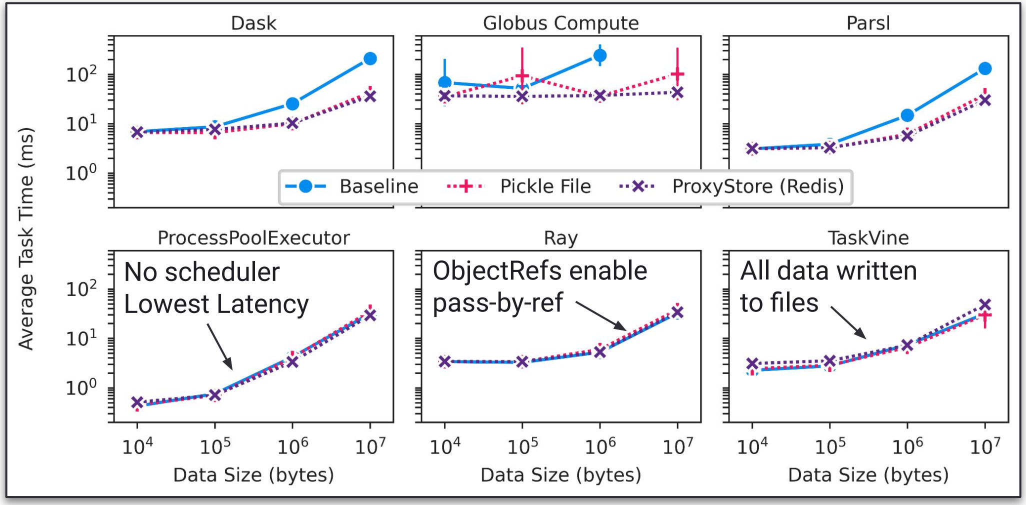
Workload

- Synthetic App – Bag of Tasks
- 32 workers and 32 concurrent tasks
- Vary input/output data size
- Record task round-trip time

Methods

- **Baseline**: Executor handles serialization and transfer
- **File**: Data pickled, written to file, and replaced with file path
- **ProxyStore**: Data is proxied, stored in Redis, and replaced with proxy object

Central **schedulers** enable advanced features but are a **bottleneck** for data transfer



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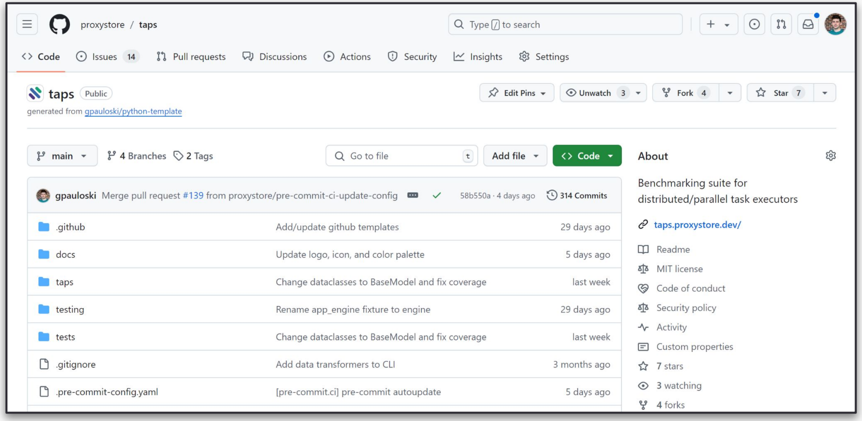
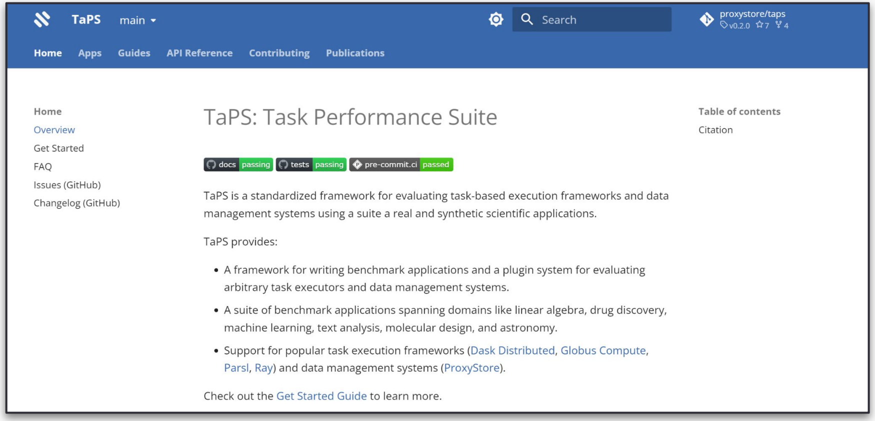
Keep Exploring — Give TaPS a Try!



github.com/proxystore/taps



taps.proxystore.dev

Want to collaborate? Reach out if you have…

- ➔ an application that could be a benchmark,
- ➔ a new execution framework,
- ➔ a data management system,
- ➔ and more!

TaPS

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J. Gregory **Pauloski**


Valerie **Hayot-Sasson**


Maxime **Gonthier**


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Questions?

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github.com/proxystore/taps/issues

Reference:

https://github.com/proxystore/taps

https://taps.proxystore.dev

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GitHub

github.com/proxystore/taps

Preprint

arxiv.org/abs/2408.07236

Slides

gregpauloski.com/#presentations