Lawrence Livermore National Laboratory

Enabling Transparent, High-Throughput Data Movement for Scientific Workflows on HPC Systems

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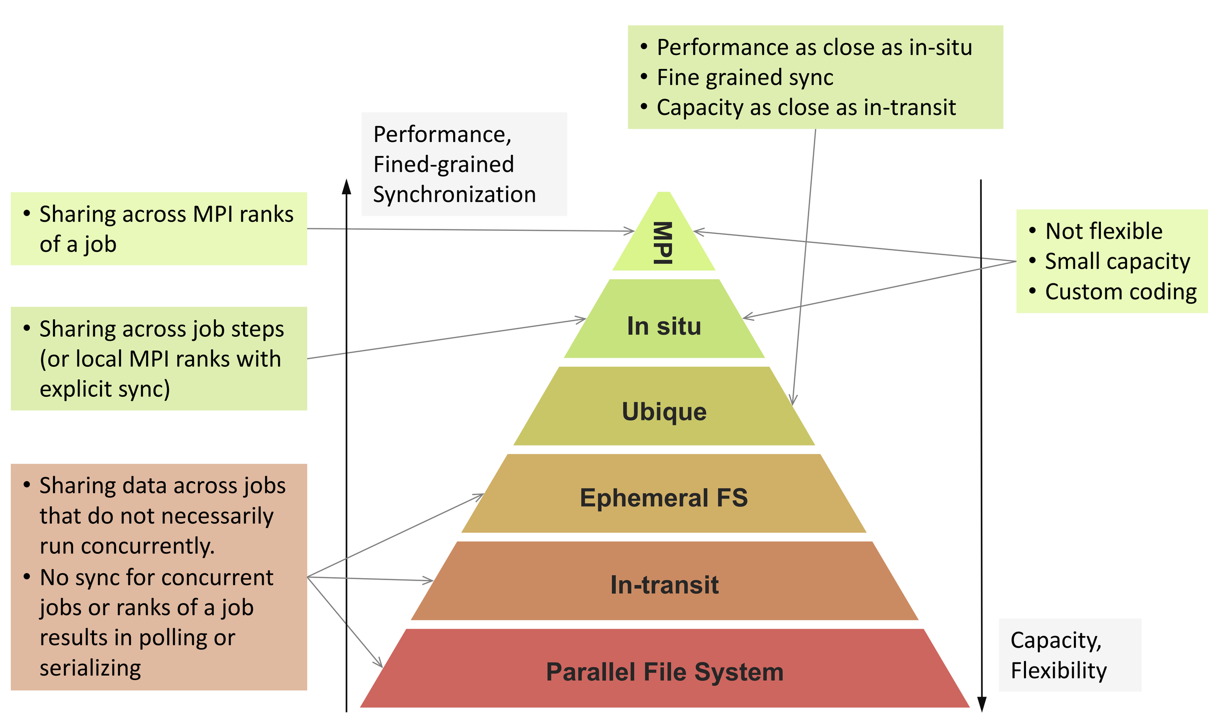
ABSTRACT

This poster presents the DYnamic and Asynchronous Data Streamliner (DYAD) middleware that provides an efficient and transparent method for data movement in scientific workflows based on the producer-consumer paradigm. We develop DYAD on top of Flux, a fully hierarchical HPC workload manager, and Unified Communication X (UCX), a unified framework for networking on HPC systems. We measure DYAD's performance with a suite of mini-apps and show how it outperforms traditional methods for data transfer while providing a high level of transparency.

CHALLENGES

There exists various approaches to resolve the **inter-task data dependence**, namely the sequential approach, which is based on a shared parallel file system (PFS), and the ***in situ*** approach [1]. However, both approaches retain one or more of the following major drawbacks:

- **Lack of synchronization support at the file/data object level**: requires workflow themselves to synchronize consumer and producer tasks to handle cases like a consumer task attempting to read a file before the producer completes its writing.
- **Poor temporal/spatial locality**: Workflows use coarse grained synchronization thereby a consumer task does not start its program execution before its dependent producer finishes its entire program execution, incurring distant temporal distance to resolve a data dependency, and each file travels a long spatial distance, missing bypass opportunities.
- **Low file metadata-operation performance**: Massive numbers of small files are often employed for emerging ML-based workflows, and hence the performance of file transfers is ultimately limited by the metadata performance of the PFS.
- **Conflict with code change requirements**: Many emerging workflows compose reusable components with minimum or no code change requirement on the pre-existing programs, and hence extensive changes needed to implement the aforementioned synchronization mechanism are often a nonstarter.



APPROACH

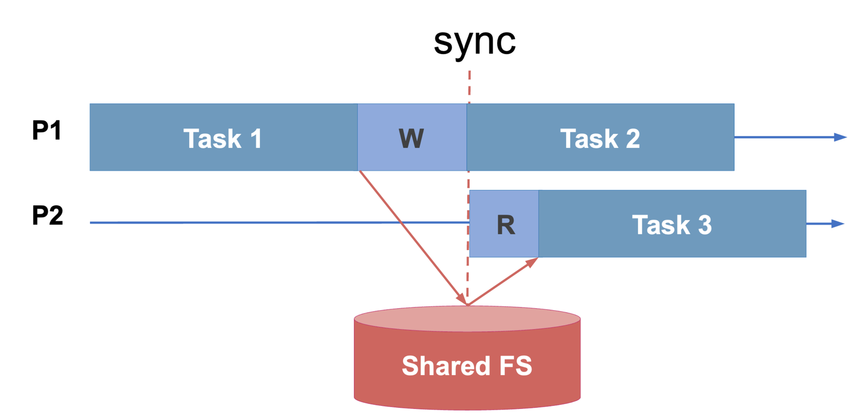
Problem: Couple an application that produces data with another that consumes the data with minimum or no code change.

```
void producer() {
   for (i=1; I <= N; i++) {
      produce(data[i])
      write(data[i]);
   }
}
void consumer() {
   for (i=1; I <= N; i++) {
      read(data[i]);
      consume(data[i])
   }
}
```

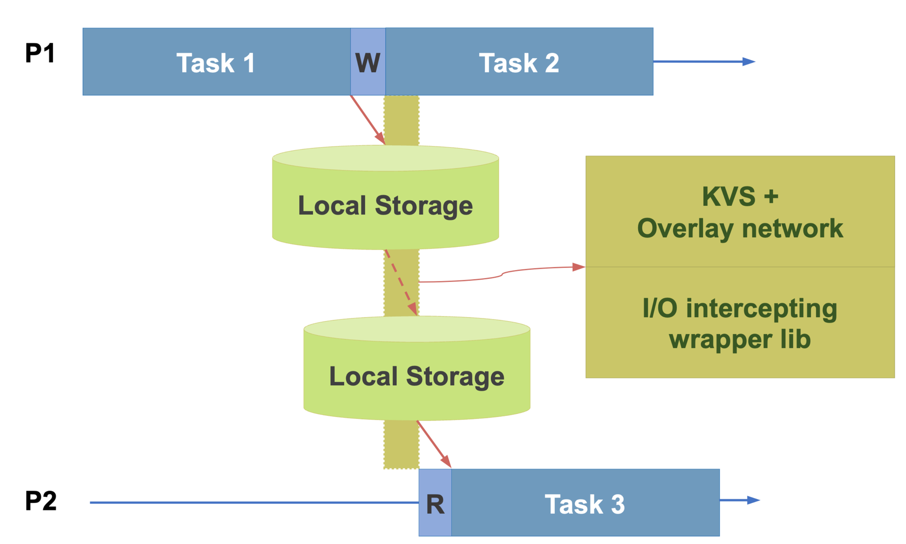
```
- description: producer task
  name: run-producer
  run:
    cmd: producer

- description: consumer task
  name: run-consumer
  run:
    cmd: consumer
    depends: [run-producer]
```

(a) Producer-consumer example (b) Maestro [2] specification in YAML

Solution 1: Sequential approach, as exemplified with Maestro, relies on a shared file system and an explicit synchronization between the end of the producer application and the start of the consumer.



Solution 2: Ubique approach [6] relies on local storages as well as transparent data transfer between storages and synchronization per shared file.



USER INTERFACE

- Running the dyad service with Flux [3]
  - `flux exec r all flux module load dyad.so /ssd/managed_dir`
- Running a user application with one of DYAD's user interfaces
  - Wrapper Library: replaces C file I/O calls with DYAD code using `LD_PRELOAD`
  - C++ Library: wraps C++ filestreams
  - Python Library: wraps Python's `open` function

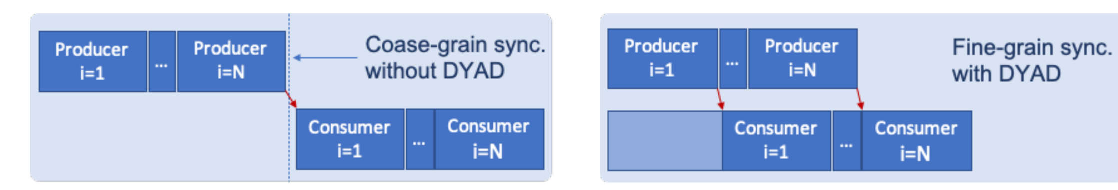
BENEFITS

No code change allows the benefits of

- Productivity (Fast construction of workflows with less effort)
- Easy debugging
- Portability (independent of any specific API other than widely used POSIX IO)

Performance benefits:

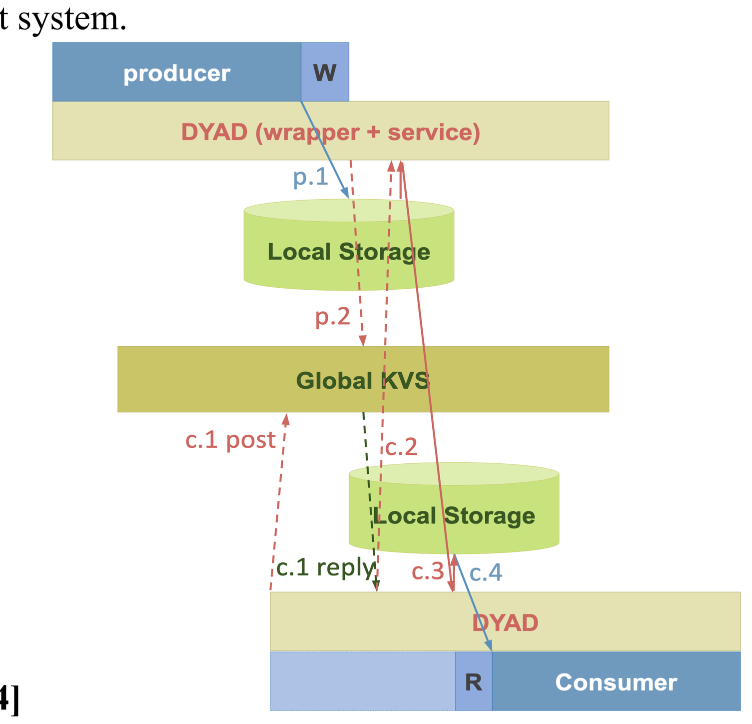
- Use of local storage enables faster accesses to storage and allows avoiding metadata operation bottleneck of PFS.
- Fine-grain file level synchronization with Ubique exposes further parallelism.



(a) Solution 1 **(b) Solution 2**

IMPLEMENTATION

DYAD: An embodiment of the Ubique model under Flux [3] resource and job management system.



DYAD [4]

- DYAD server runs on each node.
- DYAD client only intercepts I/O on files under the directory it manages.
  - If a file is on a local storage (LS), synchronize accesses and transfer it.
  - If it is on a shared storage, only synchronize accesses.

Producer

- p.1 *write(manged_dir/filepath)*
- p.2 *publish(<filepath, prod_rank>)*
  - If a file is written into ***managed_dir*** or its subdirectory, DYAD registers the filepath into the global key-value-store (KVS) of Flux.
  - KVS entry is a pair of ***filepath*** and ***prod_rank***, where prod_rank is the Flux rank of the service on the node where the producer is running on.

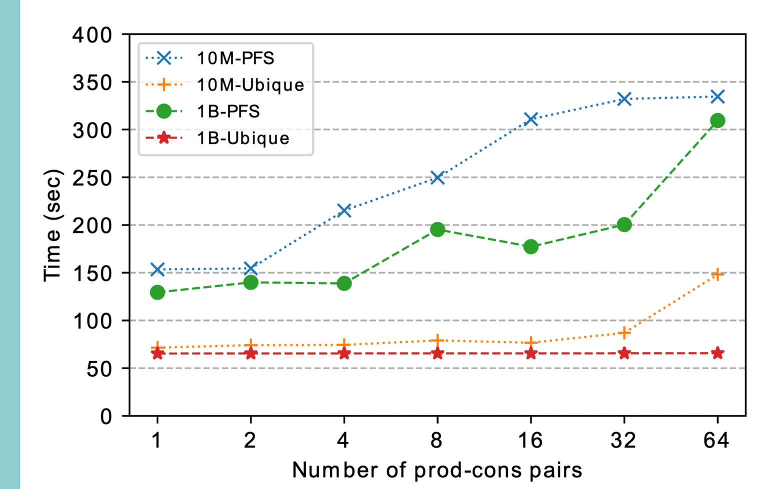
Consumer

- c.1 *query(filename)→ prod_rank*
  - Consumer queries KVS to obtain the rank of the file owner (producer). Then, blocking wait.
- c.2 *rpc_get(prod_rank, filename)*
  - Consumer asks the owner rank to transfer the file. DYAD module transfers the file to consumer using UCX. Once received, consumer stores it on LS
- c.3 make a copy of the data file on consumers LS
- c.4 *read(managed_dir/filename)*

GitHub Repo:

RESULTS

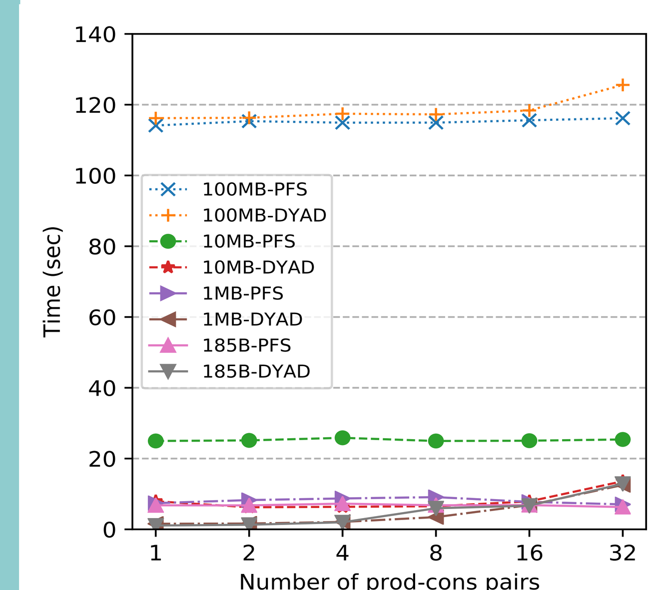
Synthetic Producer-Consumer Benchmark



Experimental setup:

- 1 second-long computation between file I/Os.
- 1 process (either producer or consumer) per node.
- Each producer-consumer pair exchanges 64 files.
- Measured on Quartz@LLNL: Intel Xeon E5-2695 v4 w/ 128 GB
- Node local storage of DYAD: tmpfs (memory)
- Parallel File System: Lustre

Molecular Dynamics-Inspired Producer-Consumer Benchmark



Experimental setup:

- Built on the Analytics4MD [5] framework
- Synthetic molecular dynamics data generation and analysis
- 1 process (either producer or consumer) per node.
- Each producer-consumer pair exchanges 64 files.
- Measured on Corona@LLNL: AMD Rome w/ 256 GB
- Node local storage of DYAD: on-node NVRAM
- Parallel File System: Lustre

CONCLUSIONS

- We present DYAD, a middleware for efficient and easy-to-use data file-sharing for scientific workflows based on the producer-consumer paradigm on HPC systems.
- We show that DYAD can speed up small- and mid-scale producer-consumer workflows up to six times compared to a sequential approach for moving data.
- In future work, we will examine DYAD's performance at larger scales and for a broader set of applications.

REFERENCES

[1] C. Docan, M. Parashar, and S. Klasky, "Dataspaces: An interaction and coordination framework for coupled simulation workflows," in ACM Intl. Symp. on High Performance Distributed Computing, 2010.

[2] Maestro Workflow Conductor, https://maestrowf.readthedocs.io/en/latest/

[3] D. H. Ahn, N. Bass et al., "Flux: Overcoming scheduling challenges for exascale workflows," Future Generation Computer Systems, vol. 110, pp. 202–213, 2020.

[4] DYAD repository: https://github.com/flux-framework/dyad

[5] M. Taufer, S. Thomas et al., "Characterizing In Situ and In Transit Analytics of Molecular Dynamics Simulations for Next-Generation Supercomputers," in IEEE eScience, 2019.

[6] J. S. Yeom, D. H. Ahn et al., "Ubique: A New Model for Untangling Inter-task Data Dependence in Complex HPC Workflows," in IEEE eScience, 2023.

ACKNOWLEDGMENTS

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