Ubique: A New Model for Untangling Inter-task Data Dependence in Complex HPC Workflows

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ABSTRACT

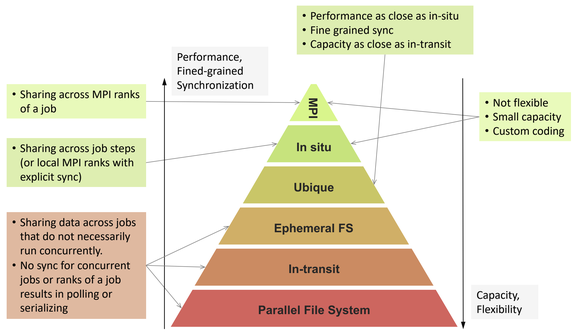
Exploiting task parallelism is getting increasingly difficult for diverse and complex scientific workflows running on High Performance Computing (HPC) systems. We argue that the difficulty rises from a void in the spectrum of existing data-transfer models for resolving inter-task data dependence within a workflow and propose a novel model, Ubique, to fill that gap.

The Ubique model combines the best from *in-transit* and *in situ* models in order for loosely coupled producer and consumer tasks to run concurrently and to resolve their data dependencies efficiently with little or no modifications to their codes, striking a balance between transparent optimization, productivity, and performance. Our preliminary evaluation suggests that Ubique can significantly outperform the parallel file system (PFS)-based model while offering transparent data transfer and synchronization which are the features lacking in many traditional models.

CHALLENGES

There exists various approaches to resolve the **inter-task data dependence**, including those based on a shared parallel file system (PFS), a ***in-transit*** model or an ***in situ*** model [1]. However, each of these approaches retains 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.
- **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.
- **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.



APPROACH

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

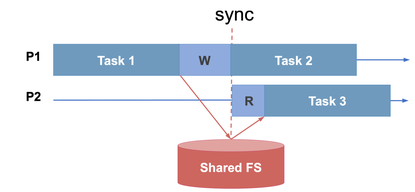
```
void producer() {
   for (i=1; I <= N; i++) {
      produce(data[i])
      write(data[i]);
   }
}
```

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

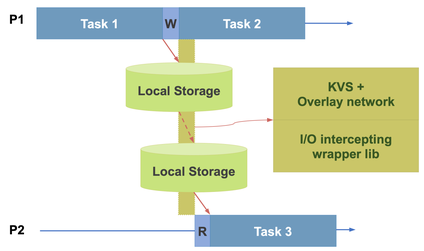
```
- description: producer task
  name: run-producer
  run:
     cmd: producer

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

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

Solution 1: Traditional 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 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 written in C with the I/O intercepting wrapper

```
LD_PRELOAD=dyad_wrap.so:${LD_PRELOAD} ./app
```

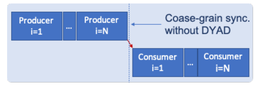
BENEFITS

No code change allows the benefits of

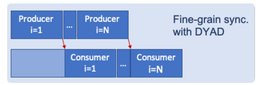
- Productivity (Fast construction of workflows with less effort)
- Easy debugging
- Portability (independent of any specific API other than widely used POSIX IO)

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.



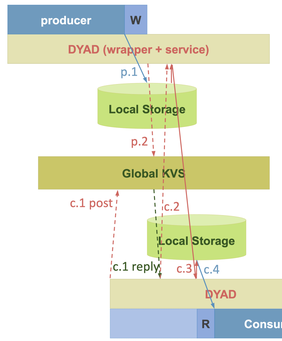
(a) Solution 1



(b) Solution 2

IMPLEMENTATION

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



DYAD [4]

- DYAD module (or service) runs on each node.
- DYAD wrapper 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

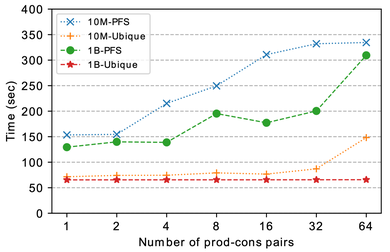
- p.1 *write(manged_dir/filepath)*
- p.2 *publish(<filepath, prod_rank>)*
  - If a file is written into ***managed_dir*** or its subdirectory, DYAD registers the filepath into the global key-value-store (KVS) of FLUX.
  - KVS entry is a pair of ***filepath*** and ***prod_rank***, where prod_rank is the 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)*
  - Ask the owner rank to transfer the file. Once received, store it on LS
- c.3 make a copy of the data file on consumers LS
- c.4 *read(managed_dir/filename)*

RESULT

From synthetic benchmark of producer-consumer pattern



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

CONCLUSIONS

- We propose Ubique, a new data file transfer model to enable modern HPC workflows to expose and exploit task-level parallelism.
- It transparently resolves data dependence between workflow tasks via fine-grained synchronization and direct data file transfers over network while avoiding persistent storage I/O bottlenecks, which are the features lacking in many traditional models.
- Our preliminary evaluation suggests that Ubique can significantly outperform the parallel file system (PFS)-based model.
- Ubique also offers enhanced productivity and portability of workflows.

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

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