# Three Practical Workflow Schedulers for Easy Maximum Parallelism

David M. Rogers<sup>†[0000-0002-5187-1768]</sup>

#### Abstract

Runtime scheduling and workflow systems are an increasingly popular algorithmic component in HPC because they allow full system utilization with relaxed synchronization requirements. There are so many special-purpose tools for task scheduling, one might wonder why more are needed. Use cases seen on the Summit supercomputer needed better integration with MPI and greater flexibility in job launch configurations. Preparation, execution, and analysis of computational chemistry simulations at the scale of tens of thousands of processors revealed three distinct workflow patterns. A separate job scheduler was implemented for each one using extremely simple and robust designs: file-based, task-list based, and bulk-synchronous. Comparing to existing methods shows unique benefits of this work, including simplicity of design, suitability for HPC centers, short startup time, and well-understood per-task overhead. All three new tools have been shown to scale to full utilization of Summit, and have been made publicly available with tests and documentation. This work presents a complete characterization of the minimum effective task granularity for efficient scheduler usage scenarios. These schedulers have the same bottlenecks, and hence similar task granularities as those reported for existing tools following comparable paradigms.

<sup>†</sup> Oak Ridge National Laboratory, Oak Ridge TN 37831, USA

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#### Abbreviations Used

API application programming interface HPChigh-performance computing DAG directed acyclic graph

HPC high-performance computing DAG directed acyclic graph DFM distributed free monoid REST representational state transfer METG minimum effective task granularity **1 Introduction**There can be no doubt that task scheduling is one of the core infrastructure components of HPC. At a system-level, an effective scheduler fills up the parallel computer with work, and obtains statistics on resource utilization. At a program-level, algorithms are constantly being re-written for task parallelism. For example, job dispatching is a key component of the OpenMP runtime, and C++ standards are expanding with parallel constructs like threads, coroutines, and futures.[1]
One of the major difficulties facing the widespread adoption of task scheduling methods is the lack of uniformity in their intended usage and user interface. This is especially important for task systems, because task completion is a synchronization event that we would ideally like to exploit for a variety of other work such as logging, network and disk I/O, and, of course, inspection of results and creation of new tasks. This requires strong guarantees that all the expected outputs of a task are visible before completion events are triggered.

come easier to use and implement. This work introduces three new scheduling implementations that provide fully functional, minimal archetypes for user interactions with workflow schedulers. The major distinctions between them come from alternative assumptions about where and how task outputs are specified. The pmake tool is file-based, and uses a single managing process to push jobs to workers. The global view of jobs allows an earliest-finish-time priority. It synchronizes based on presence or absence of output files. The dwork tool is network-service based. Worker processes interact with a task-list server to retrieve and record completion of tasks by name. Its view of the task graph lends itself to a FIFO scheduling strategy. It synchronizes through a single server that guarantees all dependencies of a task

are complete before serving that task to any worker. The mpi-list tool maintains a unique assignment of data elements to processes, so that no synchronization is needed for local operations. It targets single-program, multiple-data operations within the MPI (message-passing) paradigm of synchronization.

These concepts have all appeared before in multiple forms. What is new and novel here is that they have been stripped to their essentials and made as simple as possible. Limiting each tool to implement only a single synchronization mechanism makes the assumptions clear and simplifies the user interface, debugging process, and system installation.

Task scheduling systems are productivity tools when they are easy to use, and so fitness-for-purpose is most important. However, they can also be sources of overhead for a large computation. I quantify the overhead of each task scheduling tool in order to understand the 'minimum effective task granularity' (METG). This measure was introduced by Ref [2] to measure the overhead incurred during actual task processing. Basically, it measures (in seconds) the task difficulty needed to equally divide total execution time between scheduling overhead and actual work done on the task. Any task taking a bit longer than this will spend the majority of its time in the computation phase. They found that there are large number of scheduling systems that achieve METG values of 0.01 to 0.1 milliseconds (ms). However, general-purpose task schedulers like Spark, Dask, and Swift/T require hundreds of ms, likely due to maintaining additional job metadata.

The results section of this work will show that the underlying assumptions of the task distribution method can change the key parameters in the scaling equation. Specifically, the METG can depend on the machine size. The design of the task manager determines the functional form of that dependence. At the configurations tested here (1-6912 ranks), the METG varied between 0.5 ms and 5 seconds depending on the tool used. In practice, this means that certain types of schedulers require larger batches of work to be practical.

The tools presented here have already proven useful on several projects underway on the Summit supercomputer. including managing hundreds of molecular dynamics simulations and analysis steps pmake, [3] running docking and AI-based rescoring (dwork),[4] and summarizing results (mpi-list).[5] This work shows that, when used correctly, they achieve full parallelism with negligible run-time overhead.

Section 1.1 provides a brief classification of some popular runtime task schedulers, showing key distinctions in their implementation ideas. Section 2 presents the design of three new task schedulers, pmake, dwork, and mpi-list. Section 3 presents the details of this work's evaluation method to quantify METG. Section 4 provides numerical results, which are discussed further in sections 5 and 6.

# 1.1 Review of existing schedulers

There are multiple trade-offs implicit in the design and selection of schedulers. Ref. [6] provides a taxonomy and Ref.[6] gives an extensive feature comparison. Table 1 compares features of schedulers considered for the applications motivating this work.[3] Note that the list is heavily biased toward applications intended to run datacenters because I am interested in tracking progress of 'campaigns' in a faulttolerant way. For this work, I define a simulation campaign as a collection of many compute-intensive tasks. In some cases, the entire campaign can collectively require more resources than available from the batch scheduler (e.g. due to limits on available nodes and run-times). Task managers can achieve fault tolerance over campaigns by tracking the list of pending tasks and tasks resulting in errors. The first three columns in the table show that most workflow managers built for campaigns also provide database backends and an API to query task status. This fault tolerance comes at the cost of increased latency for tracking and assigning tasks.

Setting up and interacting with the task manager is also important. The 'Language' column shows what programming languages are available to create task graphs. Most task systems are focused tasks forming a directed acyclic graph (DAG), and interface with Python. Most scientific computing programs, however, use a mix of C, C++, Fortran, and Python, and not all computations can be expressed as a DAG. The 'Dynamic' column shows how the task manager implements updates to the task graph from the computation itself (while in-progress). Most task managers support appending tasks to the graph, but few consider this as a design feature. Some have a loop construct to explicitly support iterating a task multiple times. Fireworks allows general rewrites of the task graph, but does not provide a consistent execution semantics. Regent provides constructs to dynamically utilize hierarchical processor groups.

The last column describes the way tasks are assigned to workers. In pull-based systems, the workers request tasks from the manager. These systems are easier to setup than push-based managers, since the manager process does not need a node-list at startup. Push-based systems like Spark and Dask attempt to optimize task placement. Signac and RADICAL-Pilot use a push system so that groups of nodes can be allocated at once.

In operational terms, the three task schedulers introduced in this work, (pmake, dwork, and mpi-list) are closest to SnakeMake, RADICAL-Pilot, and py-sparkling[20], respectively. Key differentiating features of the present tools include a smaller API and better integration with the MPI-inside-batch job paradigm appropriate for Summit and Andes systems. pmake uses all resources within a single batch job, avoiding indefinite batch queue waiting times and maximizing multi-node usage. dwork has a single client and server. This relies on the user to launch clients with the appropriate resources instead of specifying them to the workflow system. Neither py-sparkling nor Spark distribute datasets over MPI ranks.

Apache Airflow, dwork, Signac/flow, SnakeMake, Fireworks, Pegasus, and Dask.distributed are all built around the basic idea of providing a central database of tasks with task-dependencies forming a DAG. Most provide a programmatic way of constructing tasks and specifying their dependent tasks. Python and yaml fit naturally into this level of abstraction because of Python's design goal as an easy shell interface and its large ecosystem of libraries. Most tasks at this level of abstraction are expected to last around tens of seconds. dwork also implements the DAG idea. It allows for dynamic tasks by implementing a 'rewrite' mechanism to add new dependency edges to a running task. This replaces the running task back into the queue to be re-run when the newly added dependencies are complete.

Resque, RADICAL-Pilot, and MetaQ do not maintain graph dependencies for tasks. Instead, tasks are expected to be trivially parallel. Resque and RADICAL-Pilot do provide the option of submitting other, follow-on, tasks. Resque tasks interface well with Ruby, since they can be yaml-serialized Ruby function code. Its intended use case is to carry out long-running tasks needed to manage files, eventually updating github's web databases. RADICAL-Pilot is intended to run Python and shell tasks. MetaQ provides a Slurm-like syntax for specifying resources. It is intended to bundle multiple batch-queue jobs into a single batch job to reduce overall queue wait times and increase (outer) batch job sizes.

Spark and mpi-list are unique in that they do not use the DAG-of-tasks concept. Instead, work distribution is based on a globally known assignment of data to processors where computations are carried out. Because of this, its programming model is bulk-synchronous single-program, multiple data. Their method of task-addition is described as 'interactive', since the program dynamically chooses its execution path at the top-level of execution.

Regent and Parsec target HPC workloads. These are not expected to out-live a job allocation, so do not have database backends. They also employ special distribution strategies to optimize for minimal latency between tasks. Specifically, both Regent and Parsec use a shared execution model where every worker explicitly models (at least) the local task graph and its mapping to compute resources. Leaving out a central database reduces communication latencies.

Compared to the existing runtime task scheduling systems, pmake fits into the class of file-directed, make-like job schedulers. This design decision is a natural parallel to the Make build tool. The mpi-list tool follows the general ideas of Spark, but is more compatible with HPC environments. In particular, it is based on mpi4py[21], simplifying job launch. Instead of a resilient distributed dataset holding a list of partitions, mpi-list uses a DFM, which holds a list of arbitrary objects. This makes it operate equally well holding lists of plain integers, numpy or cupy arrays or pandas DataFrames. The DAG-of-tasks concept underlying dwork is not unique. Instead, what dwork provides is a less obtrusive management layer. The only purpose of dwork is to define a network API for creating and assigning tasks. This borrows a design idea from resque, and provides a much simpler framework for feature expansion than other available options.

# 2 Description of the Design and User Interface

This section describes the design and implementation of three separate task schedulers. The designs differ based on their intended use pattern.

#### 2.1 pmake

Pmake is a parallel version of the 'Makefile' concept. Every task corresponds to one or more output files, which determine whether the task needs to be run. Rules describe

	Target	Query	Persistence	Language	Dynamic	Push/Pull
Apache Airflow[7]	datactr	REST/CLI	SQL	Py	modify globals[8]	pull from broker
Apache Spark[9]	datactr	CLI	checkpoint	Scala/Py/R/Java	interactive	push
${\tt mpi-list}^*$	datactr	no	no	Py	interactive	push
Resque[10]	datactr	REST	Redis	Ruby	append	pull
RADICAL-Pilot[11]	modeling	?	Mongo	Py	append	push
MetaQ[12]	modeling	no	file	shell	no	push
Signac/flow[13]	modeling	$\mathrm{CLI}/\mathrm{WebUI}$	file or Mongo	Py	append	push
SnakeMake[14]	modeling	CLI	file	shell/Py	no	push
pmake*	modeling	CLI	file	shell	no	push
Fireworks[15]	modeling	$\mathrm{CLI}/\mathrm{WebUI}$	Mongo	Py	rewrite	pull
Pegasus[16]	modeling	$\mathrm{CLI}/\mathrm{WebUI}$	$\operatorname{SQL}$	DSL/Py	?	push
dwork*	modeling	$\rm ZMQ/CLI$	TKRZW	Proto+ZMQ	replace	pull
Dask.distributed[17]	analytics	Py API	no	Py	?	push/steal
Regent[18]	HPC	no	no	Regent	hierarchical	shared
Parsec[19]	HPC	no	no	DSL	loop	shared

Table 1: Feature comparison of present work (\*) with popular workflow schedulers. Missing entries (?) indicate features that were not able to be determined from the tool's documentation. datactr: cloud or HPC datacenters, REST: HTTP interface, CLI: command-line interface, WebUI: web user interface, Py: Python, DSL: domain-specific language

how to create output files from input files. Pmake is a single Python program that reads a list of rules and a list of target files and runs all tasks in the task-graph.

Because the pmake process views the entire task graph, it is able to assign earliest start times to all tasks by traversing the DAG from leaf (immediately executable) to root (most dependent) nodes. Instead of using the time directly, it uses the total node-hours consumed by a task and all its transitive successors to assign a priority to every task. Then, it uses a greedy strategy to choose the highest priority task from those runnable at each time point.

In place of the Makefile, pmake employs a rules.yaml file. An example rules.yaml is shown in listing 1a. The two rules form a sequence simulate  $\rightarrow$  analyze, which eventually produces files like an\_1.npy, an\_2.npy, and so on. In operation, pmake will generate simulate.n.sh from the setup and script section and execute it in the background sending its stderr and stdout to simulate.n.log. It continues until it runs out of available allocated compute nodes. Exiting scripts release their nodes. Scripts exiting with a zero-return value trigger any waiting rules.

There are several important design decisions shown from this example. Rules have extra meta-data compared to standard makefiles: *i*) a resource set, *ii*) a list of multiple input and output files, *iii*) a setup script, and *iv*) automatic creation of an {mpirun} command, which expands to the appropriate **srun** or **jsrun**, depending on whether Slurm or LSF scheduler is used. Also, the syntax for variable substitution is determined by Python's **format()** function. For rules that can make multiple output files, one variable is allowed, and is defined by matching on names in the **out** section.

A resource set specifies a division of the allocated nodes for a job into equally-sized resources – each with a fixed number of CPUs and GPUs. Usually, one MPI rank is assigned to each resource set, but it is also possible to set ranks = R to launch R MPI ranks on each resource set instead. Resources in pmake also include time (specified in minutes). This is used by pmake to prioritize tasks ready to be run on the machine by estimating earliest-finish time.

The inp section lists files required before the rule can be triggered. Like make, pmake stops searching for rules when it finds all the files needed to build its outputs. Inputs can also be specified using a loop directive (not shown), which lists input files generated by filling in a template with a Python iterable.

Often the same set of operations are run across multiple problem instances. Listing 1b shows a targets.yaml file. This file lists out the top-level targets the user would like to build. Each target has an arbitrary name and attributes available to be substituted into rules that run for the target. Reserved keywords for the target are dirname, out, and loop. All the target files are relative to the dirname. The out and loop file lists have the same format as for inputs to rules.

When a rule is run, its setup and job-scripts are concatenated together and pre-pended by a set -e and a cd into the target's dirname. The result is written to a shell script 'rulename.n.sh' named after the rule name and its template variable, n, (if present). That shell script is executed locally by a call to popen, and its output stored in a logfile, also named 'rulename.n.log' after the rule.

The use of Python's format function allows Python code to be spliced into the script. Substitution happens in order from targets to rules, so that variable references will only work for variables declared earlier. The order is: *i*) members of the target (other than loop – these are first, so not substituted), *ii*) variables in the loop directive are substituted sequentially, *iii*) members of the rule (other than script), *iv*) script directive (which also gets 'mpirun' defined from the scheduler). One drawback is that braces ({}) must be escaped.

# 2.2 dwork

dwork is a client/server API implementing a bag of tasks. Because tasks can have dependencies, these tasks can form a directed acyclic graph (DAG). When tasks insert new tasks, the computation expressed by the graph can create loops. Table 2 lists the key messages implemented by the dwork API. For the implementation, each of these messages is encoded in Google protocol buffers[22] and passed through ZeroMQ.[23]

Because the server is not assumed to have a complete view of the task graph, it uses a first-in-first-out assignment strategy for tasks. Workers that request a task are served with the oldest task inserted into the database that is ready to run (based on completed dependencies). On the other hand, tasks that are re-inserted back into the graph are added to the front of the priority queue. This double-ended queue setup is exactly the same one used for work-stealing, where remote workers resume the 'oldest' task, while the local processor executes the 'newest'.

The server for dwork (dhub) uses a TKRZW[24] database to store the task graph. Like Redis[25] it can save and restore the database to file for persistent state. Unlike Redis, its API is centered around creating tasks and assignments. The task database internally contains only two tables: a table of join counters and successors for each task and a table of task metadata (name, originator, etc.) for each task. Other run-time information, such as the list of tasks ready to run, can be generated from these tables on startup.

```
simulate:
  resources: {time: 120, nrs: 10, cpu: 42, gpu: 6}
  inp:
    param: "\{n\}.param"
  out:
    trj: "{n}.trj"
 setup: module load cuda
  script: |
    {mpirun} simulate {inp[param]} out{[trj]}
analyze:
  resources: {time: 10, nrs: 1, cpu: 1}
  inp:
        "{n}.trj"
    trj:
 out:
   npy: an_{-}\{n\}.npy"
  setup: module load Python/3
  script:
    {mpirun} Python compute_averages.py {inp[trj]} {out[npy]}
```

(a) Example rules.yaml file with make-rules for executing parallel programs.

sim1: dirname: System1 out: npy: "an\_0.npy" loop: n: "range(1,11)" tgt: npy: "an\_{n}.npy"

(b) Example targets.yaml file listing out high-level output files.

Fig. 1: Pmake program inputs for a typical simulate, then analyze workflow. This workflow creates System1/an\_0.npy, ..., System1/an\_10.npy by running the simulate and analyze rules multiple times from the System1 directory.

I also provide a command-line tool (dquery) as an example client that can interact with the API from shell scripts. Usually, users write their own software to interact with dhub. This works well in practice, since tasks are software anyway, and protobuf and ZeroMQ are supported in a very wide variety of programming languages.

The API is consumed both by users of the system (who create tasks), and processing nodes (who call Steal, Complete and Transfer). Figure 2 provides pseudocode for the operation of the client and server around these API calls. Internally, the scheduler maintains the successors of every task, along with a join-counter. The join counter goes to zero when all the task's dependencies are marked completed. It also maintains a mapping from Worker-s to sets of Task-s assigned to that worker. The scheduler will not assign a task (via responding to Steal) unless all of the task's dependencies have been marked completed.

If workers have unique hostnames, calls to 'Exit' can be run by the worker or by the user to recover from a node failure or abort. When receiving such a notification, the queuing system moves tasks assigned to the exited worker back into the pool of ready tasks.

This implementation signals completion of the task graph by responding three different ways to 'Steal'. Usually, a task is provided to the worker. In case no tasks are ready, the manager responds with a 'NotFound' message. In case all tasks are complete, the manager responds with 'Exit.'

Valid task graphs do not contain cycles. This is mostly guaranteed by the syntax for creating tasks. The only potential way to add a cycle is during 'Transfer'. The transfer operation moves a task back from a worker (where it was assigned) to the manager. New dependencies (prerequisites) can be added to the task at this point. If the new dependencies are waiting for a task that transitively depends on the transferred Task itself, this is a user-error that creates deadlock. Observationally, such tasks will never enter the 'ready' state, and thus never be served to workers.

#### 2.3 mpi-list

The mpi-list tool is a Python package that provides a functional API for manipulating lists. The syntax and design is inspired by Spark,[9] although the startup and communication mechanisms of mpi-list are purely based on mpi4py.[21] Because all MPI ranks execute the same operations on their local portion of the dataset, its scheduling model is bulk-synchronous-parallel.

Mpi-list provides only two classes - a 'Context' to hold the MPI communicator information, and a 'DFM' object to represent distributed lists. DFM stands for distributed free monoid. The 'DFM' object stores only the set of list elements local to each rank. The global list is logically maintained in an ordered state, with a contiguous and ascending subset of the list assigned to each rank. New 'DFM' objects are created with 'Context.iterates(N)', which creates a distributed list of N sequential integers. Rank p of P stores the subsequence starting at  $p \operatorname{int}(N/P) + \min(p, N \mod P)$ .

It is not usually necessary to index local list elements directly. Instead, operations like 'DFM.map(f)'. Create new lists by applying the function, f, to each list element. There are also functions for both full reduction and parallel prefix-scan reduction. To move elements between ranks, a 'DFM.repartition' and 'DFM.group' are implemented.

The 'repartition' function does not simply move list elements, but instead treats each list element as a complex list-like datastructure containing multiple records. This is because the intended usage of mpi-list is to store numpy or cupy arrays, or pandas dataframes. The repartition function thus requires three functions: one reporting the length of the stored objects, one able to subdivide the object into multiple chunks, and another able to combine multiple chunks together again. Obviously, the mpi-list implementation is handling the mundane counting and communication tasks.

Query	Parameter	Response	Description
Create	Task, [Task]	-	Create a new task with the given de-
			pendencies.
Steal	Worker	Task?   Exit	Deque (steal) a ready task to be run
			by the worker.
Complete	Worker, Task	-	Notify the scheduler that a task is
			complete.
Transfer	Worker, [Task]	-	Replace the task and add new de-
			pendencies.
Exit	Worker	-	Notify the queuing system that a
			processing device is down.

Table 2: Minimal API for maintaining a distributed a task list. Workers send these queries to the task manager, which replies with the response. Repetitions of zero or more entries (lists) are denoted by brackets. The data-type for Worker is implemented as a string, while Tasks are defined as protocol buffer messages to allow passing additional meta-data about the task.





Fig. 2: Client/Server Interaction API Implementation in dwork. Production client code would use an assembly-line pattern to overlap these 4 steps.

```
from mpi_list import Context
import xarray as xr
C = Context()
dfm = C . iterates (N) \setminus
             . flatMap( lambda n: read_scored(data, prot, n) ) \
              map( best_scores )
n = dfm.len()
if C.rank == 0:
    print (f"Read_{n}_pq_files_to_{C.procs}_processes_in_{t1-t0}_secs.")
ret = dfm . map(stat) . collect()
if C.rank == 0:
    print(f"Collected_stats_to_rank_0_in_{t3-t2}_secs.")
    df = pd.concat(ret)
                        "summary.pq")
    df.to_parquet(out /
    lo = df . loc ['min']
    hi = df. loc['max']
# broadcast histogram parameters
lo, hi = C.comm.bcast((lo, hi), root=0)
H = Hist(lo, hi, 301, 201)
ret = dfm . map( lambda df: H.his2d(df, 'score', 'r3') ) \
          . reduce ( npsum , 0 )
if C.rank == 0:
    print(f"Collected_histogram1_in_{{t3-t2}_secs.")
    ret.to_netcdf(str(out / "score_rf3.nc"))
```

Fig. 3: Production code snippet showing use of mpi-list to read a dataset of parquet files and create a 2D histogram in parallel. This example read 2592 parquet files (80 gigabytes compressed) to 320 processes (20 nodes of OLCF Andes) in 4.0 seconds, collected stats in 1.5 seconds, then output its histogram in 0.4 seconds.

Similarly, the 'group' function requires, as input, a function to turn a stored object into a dictionary mapping destination list indices to lists of objects that should be sent to that index.mpi-list moves all the data to its newly determined MPI rank, and calls the user's combination function on each new index to re-form the list back into the final output object.

Mpi-list is released in the pypi package index, and contains full documentation and functionality tests.

# 3 Evaluation Method

Tools for managing launching and logging of tasks can be measured for performance efficiency by quantifying the overhead with respect to sequentially running all tasks directly on a single compute resource. Sometimes, this overhead can vary when computational resources are actually doing work - and so it can be helpful to measure the overhead during actual task processing. The 'minimum effective task granularity' (METG) has been introduced as a descriptive measure in this case.[2] Basically, it measures (in units of seconds) the task difficulty needed to equally divide observed run-time between scheduling overhead and actual work done on the task. If the average execution time per task equals the METG, then the total run-time (execution plus overhead) will be twice the number of tasks times the METG.

In practice, the effect of overhead is negligible when tasks are a few times larger than the METG. The METG gives a helpful guideline when dividing up work, since in many cases task sizes can be arranged to be larger than the METG. Also, the typical task size provides an estimate of the computational idle time caused at the completion of a sequence of tasks. All the task managers here operate inside a Slurm or LSF job allocation. Hence, out of the resources allocated to the job, all but one task's worth could remain idle for this time.

Although the task schedulers presented here were first put to production use on computational chemistry research with mixed CPU/GPU workloads, [3,4,5] the nonuniformity of those tasks prevent quantitative comparison.

This work presents a standard, synthetic benchmark to highlight overheads. I chose GPU-intensive matrix multiplication because of its importance to applications in highperformance computing. There, large (often machine-size) matrices are divided into tiles to distribute the data and computational work among all available resources. I apply the three schedulers here to compute a series of  $A^T B$  operations, where A and B are single-precision floating point matrices with sizes between 256 and 8192. This operation appears very often as a building block of linear algebra calculations like computation of the wavefunction overlap matrix,  $S = \psi^{\dagger} \psi$ , in quantum mechanics.[26,27] In those applications,  $\psi$  may consist of hundreds of thousands of tiles like A and B, giving rise to millions of tasks. In these workflows, however, neglect the hypothetical communication steps needed to sum the results in computing S.

Each task management system was benchmarked using a weak-scaling methodology – where number of tasks scaled with processors. The scale was set to 1024 total kernel executions per rank. Every run used 1 MPI rank per GPU, except for baseline runs intended to determine the minimum compute time needed to run the kernel itself (which used only 1 GPU). For pmake and dwork, tasks consisted of 256 iterations of the matrix-multiplication kernel. For mpi-list, one single list containing all problems was created, and then the kernel was run inside a map-function. In practice, this allowed each rank to run its 1024 assigned kernel runs inside a for-loop.

Note that this division means that all workflow systems encounter the startup costs of spawning MPI jobs, initializing the GPU and allocating memory only once – except for pmake. pmake encounters the batch spawn and 'alloc' cost four times per rank. These costs cannot reliably be overlapped with computation, and determine pmake's METG.

mpi-list, on the other hand, has a METG determined entirely by imbalance in execution times. Since every process runs exactly 1024 kernels, processes that get interrupted or have slower than usual GPU accesses will hold back progress on all the other ranks. Its METG is thus determined by the point at which idle time (slowest minus fastest completion) equals the ideal task completion time. In other words, the METG for mpi-list is the "slowest minus fastest" completion time per task.

For dwork, the overhead per-task comes from receiving its next task via communication with the task database. Thus, its METG is the latency time for accessing the database *multiplied by* the number of MPI ranks. The latter multiplication happens because the database must serve every rank with a task at a rate faster than the time needed for one worker to complete a single task in order to keep that worker busy.

Table 3 lists the software and dependency library versions for the scheduling tools tested in this work. The calls to cublas-sgemm were made via blaspp for pmake and dwork, or via cupy for mpi-list.

Package	Version
pmake	${\rm commit}~05{\rm f}727$
blaspp[28]	2021.04.01
cuda	11.2.0

(a) Software used by pmake and its kernel.

Package	Version
dwork	$\operatorname{commit}$ 88ebb1
zeromq	4.3.3
cppzmq	4.7.1
protobuf-cpp	3.14.0
TKRZW	0.9.3
blaspp[28]	2021.04.01
cuda	11.2.0

(b) Software used dwork and its kernel.

Package	Version
mpi-list	0.3
Python	3.7.10
mpi4py	3.0.3
cupy	8.5.0
cuda	10.1.243

(c) Software used by mpi-list and its kernel.

### Table 3

Tests were conducted on the Summit supercomputer. Each summit node has two sockets, each socket has 3 NVIDIA(R) V100 GPUs and 21 usable IBM power9 processor cores. Software versions are listed in Table 3.

# 4 Scaling Results

Fig. 4 shows computational efficiency (GFlops) of the task systems as a function of the block size. All task systems achieve peak theoretical efficiency for the hardware (14 teraflops per GPU in single-precision). This should always be achieved when the problem sizes are large enough so that computation time is much larger than any other overhead time per calculation. However, the maximum efficiency is not achieved for small tile-sizes. This is partially because of the GPU and call path to the blas library itself, and partially because of the overhead of the schedulers.

Figure 4(upper) hides potential sources of overhead that create a difference between the single-GPU run time and the parallel, task-scheduled run time. Thus, all further plots are of efficiency relative to single-GPU compute time, as is done in the lower part of Fig. 4. This measure highlights losses due to task scheduling, and ignores losses due to tile-sizes that don't saturate the GPU or (for Python) overcome the function call overhead. The measure serves to normalize the execution time across frameworks because there are small differences in initialization and multiplication time (notably mpi\_list calls the cupy library). The resulting plots highlight scheduler overhead instead of these details. The lower portion of Figure 4 reproduces the minimum effective task granularity (METG) plot of Ref. [2]. Computational efficiency, plotted on the vertical axis, is defined as ideal divided by actual per-task execution time. The horizontal axis is the task's ideal, single GPU time. The METG is defined as the task size where computation time equals half the total execution time per task. It is visible as the sharp increase in efficiency at a particular task size. This task size is helpful to state in terms of the ideal, 'single-GPU' execution time, as we have done here. Note that, for **pmake** and **dwork**, one task is defined as 256 iterations of the multiplication kernel.

Figure 5 shows the breakdown of time spent per task when running the test workflow. Each of the three runtime scheduling tools have different sources of per-task overhead. The pmake tool launches job steps during a running allocation – and so incurs both overhead from the job step launch (jsrun), and from startup tasks of the job itself (alloc). Neither of these tasks can be overlapped with computation easily. The dwork tool only stops work to request a new task from the server, and to record completion (communication). These two can be effectively overlapped with computation. The mpi-list kernel launches occur locally, so the only overhead is at synchronization points in the code. The 'sync' time measures this end-of-job synchronization. It is equivalent to the time difference between the fastest possible and slowest encountered run-times per rank.

Table 4 summarizes scaling measurements of these overhead components. Job step launch times increase roughly logarithmically with the number of MPI ranks. Task startup (GPU memory allocation) is constant independent of the job size or tile size. Communication time only appears in dwork when computation time is too small to hide it. For mpi-list, the METG equals the disparity between fast and slow computation times. This is shown by the synchronization latency column. It is slowly increasing with number of ranks. Synchronization latency is indirectly measured for mpi-list by subtracting the completion time from the 1-GPU program completion time.

Based on the performance at 846 ranks, the METG for mpi-list, dwork and pmake are 0.3, 25, and 4500, milliseconds, respectively. These can be compared to the results in Fig. 9 of Ref. [2]. There, 864 ranks correspond to between 16 and 32 nodes. Although the interconnect and processor hardware are different, the schedulers in that work fall into two classes – those with METG between 0.01 and 10 milliseconds (Chapel, Charm++, MPI, OpenMP task, OpmSS, PaRSEC, Regent, StarPU, TensorFlow, X10), and those with more than 1000 (Spark, Swift/T and Dask). Interestingly, this work's Spark-like mpi-list has the best performance, probably due to the lack of file I/O. dwork falls in-between the two groups, and pmake is in the second group.

The bulk of **pmake**'s waiting time is attributable to the startup time for executing the 'jsrun' command, which allocates a group of processors to execute an MPI program in parallel. We can see that this increase in the METG is due to an approximately logarithmically increasing task-job launch times.

For dwork, the METG is negligible on a single MPI rank, but increases proportional to the number of ranks. The relevant number from Table 4 is the 23 microseconds needed for the Steal/Complete API calls.

Unfortunately, its METG scales linearly with the number of concurrent compute ranks. For dwork, the maximum communication value is achieved by a kernel that does no work. In that case, the server is the bottleneck, and the time equals the total number of tasks assigned times the round-trip time of the network API per per-task. I have used a 2-level forwarding tree, where each rack of 18 Summit nodes communicates with a rack-leader. The rack lead-



Fig. 4: Absolute (upper) and relative (lower) computational efficiency per GPU measured using total time the workflow scheduler spends in its compute phase. One-time workflow startup phases for each are not present in this figure, but are listed Table 4.

$\operatorname{ranks}$	jsrun t	ime	alloc	<b>comm</b> (per task)	sync time per 1024 tasks	Python alloc	Python imports d	work connection
6	0	0.987	1.81	$23\mu$	0.09	2.23	1.05	1.54
60	1		1.81	$23\mu$	0.17	2.23	0.55	-
864	2	2.336	1.81	$23\mu$	0.33	2.23	2.82	2.74
6912	3	3.823	1.81	$23\mu$	0.47	2.23	26.65	13.32

Table 4: All data are times in seconds. The symbol  $\mu$  denotes a factor of  $10^{-6}$ . Column headers in bold font are costs incurred per-task (depending on the workflow tool). Constant values were averaged over all test runs because their timings did have significant run-to-run variation. Other columns are useful measures of tasking system startup time.



(c)  $6912 \ {\rm ranks}$  (1152 node) calculation.

Fig. 5: Pie-charts showing time breakdown between computation and each overhead cost for each scheduling tool (yaxis). Increasing matrix tile-sizes (x-axis) provide enough computation to overwhelm tasking overheads. METG can be seen as the point where the computation occupies more than half the time. Note that for **pmake** and **dwork**, each task carries out 256 matrix multiplications, so only four tasks are sent to each rank during a run. **pmake** shows sync-time for large runs because each pmake-task occupies 864 ranks. ers forwards all messages to a single task server running on the job's launch node. As the number of ranks increases, the communication time measured is this two-hop time.

#### 5 Discussion

The **pmake** tool provides a makefile-like syntax to run a series of **srun** or **jsrun** launches, as if they had been typed into a job-script directly. It's scaling behavior is a direct consequence of this choice. Because job launch can take tens of seconds, tasks must take at least this long in order to make effective use of the machine with this approach. This is usually the case when bundling together many jobs that would otherwise have been run on their own as isolated batch scripts. Scanning file presence and constructing a task graph can cause delays too, but are generally worthwhile because they can avoid duplicating work.

The dwork tool is built around a client/server model. Its task dispatch latency shows typical behavior following from this model. Message transfer rates using ZeroMQ[23] and hash-table entry read/write rates form lower bounds on the latency. I have avoided additional costs deriving from establishing TCP connections by establishing a tree-shaped message forwarding chain. I have added additional costs by wrapping transmitted tasks and messages into Google protocol buffers.[22] All of these choices combine to a measured cost of about 23 microseconds latency per task.

Although 23 microseconds of latency seems very small, this number means that only 44,000 tasks can be distributed to all workers per second. For a job with 44,000 MPI ranks, every task must then last at least one second in order to achieve full utilization. Even then, receiving a response could take half a second. This waiting time can be hidden by overlapping computation and communication, which I have implemented in the client. With overlapping, the task granularity is controlled by the task manager's maximum rate of dispatching jobs.

Two simple strategies are worth pursuing for increasing task dispatch rates further. The first is sending multiple tasks per 'Steal' request. I have already implemented this as a separate 'Steal n' request. The second is to replicate the server by creating multiple task databases that distribute tasks among themselves. I have designed the API to adapt to this pattern in the future, since delegating a task to another task database is logically the same as assigning it to a worker.

The last new task manager, mpi-list, has characteristics that follow from the Spark paradigm. Execution happens where data elements sit, and each process maintains its own list of local data elements. It is not suited to general task graphs. Instead, it works best on map-reduce type operations over datasets that can fit in the machine's memory. mpi-list has the smallest latency per task because our tasks do not include file operations. In my implementation, job-launch and network communication is based on MPI, making it easy to use on HPC systems. I observed a moderately large startup time for the initial launch of Python. This is not a per-task cost, but it is troubling that it increases with MPI ranks. Since this is likely due to I/O overhead from all ranks importing libraries on startup, future work should investigate using the spindle tool to reduce this cost.[29]

All of the task latencies observed for workflow scheduling systems presented in this work are on par with similar measurements in the literature. mpi-list has a latency of 0.3 ms, entirely due to barrier synchronization costs. This is slightly above the fastest schedulers from Ref. [2] because the synchronization is global, and not point-to-point. The METG for mpi-list is the largest, around 1-5 seconds. Even still, this is comparable to the smallest METG observed in Ref. [2] for the Spark, Dask, or Swift/T workflow systems. dwork has an overhead of 1 second at the largest node counts, comparable or smaller to that measured in Ref. [2] for Regent, StarPU, and Parsec.

Although the METG sets a strong-scaling limit, there are many important features for workflow scheduling systems including flexible user interface, reproducibility and tracking, ease of installation, and simplicity.[30] These multiple trade-offs necessitate making situation-specific and qualitative comparisons.

# 6 Conclusions

This work has successfully implemented and used in production several task managers for distributing asynchronous, parallel work. All three are very well suited for HPC centers with batch systems and MPI. Arguably, one of their greatest advantages is the simplicity of the implementation and user interface. The conditions under which each of the systems will execute a task are straightforward. Task tracking is not complicated, and the minimum effective task granularity is well-characterized.

Each of these scheduling systems serves as a base of useful functionality which can be modified for more efficient and specialized uses in the future. The pmake scheduler is very similar to the more full-featured SnakeMake[14], so pmake's idea of specifying a parallel resource set and machine-dependent substitions for {mpirun} can be adopted into that code. The mpi-list code seems to fill a new niche for Spark-like computations inside MPI. Nevertheless, it can be limited by memory bounds on large datasets. Further work can eliminate this issue without substantial changes to mpi-list itself by loading wrappers for the data elements that maintain the data on disk except during processing.

The dwork client/server model can be substantially expanded to include features like: 1. separate pools of work with independent servers (trivial), 2. forwarding of messages to maintain constant open connections per rank (implemented in the code released with this article), 3. more comprehensive display and interactivity with the task queue (moderate), 4. shared responsibility for handing out tasks, sharded between multiple servers (moderate), 5. advertisement of shared-memory access methods for intermediate results (advanced). Most of these features (when needed) would reduce overall task latency times and further increase scalability.

Interestingly, the minimum effective task granularity of all three dynamic scheduling tools follows different scaling laws. The pmake tool launches tasks in the background, but every task incurs startup costs from the scheduler's resource allocation and from the program startup itself. Its METG is thus equal to the job startup costs. dwork pushes job information to running clients, so the startup costs become negligible over long runs. Instead, its METG comes from the overhead of communicating the 'next ready' task. That overhead scales with the number of concurrent workers as long as a single-task-server design is used. So, its METG is the per-task latency times the number of workers. The mpi-list system apparently has no waiting time for the next instruction. However, it does have synchronization points and uses statically assigned work items. Thus, its METG is equal to the difference in run-times between 'fastest' and 'slowest' concurrent worker. That difference depends on the number of data elements processed, and is the subject of the study of extreme value distributions.[31]

When presented with these interfaces, task management appears easy. Difficulties in most implementations come from additional design requirements. For example, building a domain-specific interface requires associating additional information with each task. Preventing duplication of tasks can require external methods to determine the status of completed tasks. Specializing tasks to run on specific hardware or at coordinated times also requires some external delegation or synchronization mechanism.

This work's contributions uncouple the task schedulers from all of these concerns. Doing so achieves a simpler and more flexible design. For some problems, however, it leaves practical implementation issues unresolved. In particular, the work does not addressed the data lifecycle management issue. In OpenMP, Quark, StarPU, Parsec, and their predecessors, tasks are associated with in- and out- memory pointers. This requires tracking the association from data locations to tasks. Distributed memory runtime systems often add the further step of copying data to local resources before execution can start. Solutions like distributed caching filesystems and tuple-spaces have been designed to address this issue.[32]

Each of the issues above have multiple potential solutions with different trade-offs. This strategy allows the user to make their own implementation choices. It reduces the complexity of the task manager and usually also the user code. I have shown that this approach has latency overhead on the order of 23 milliseconds when under heavy load and can create and deque one million task in about a minute – competitive with task schedulers designed for HPC workloads.

This work does not provide a single solution to synchronization and coordination mechanisms. Instead, we are left with two opposing ideas. Task graphs are functional, expressing every part of the data flow from task to task, and tracking progress by pulling data from a collective memory. Bulk-synchronous operations on data are imperative, prescribing precisely what each processor should do. These track progress by a global instruction counter. One middleway that has been left unexplored is to earmark certain tasks for compatible locations and separately implement a rendezvous mechanism to synchronize the start-time of those tasks.

Overall, these tools provide a usable, versatile way to manage scientific simulation campaigns outside the batch scheduler. This brings scaling benefits, bringing down the time and effort needed to run multiple inter-related calculations. Their unique features are simplicity of design, suitability for HPC centers, very short startup time, and well-understood per-task overhead.

# Availability

The tools described in this work have been made available under open-source licenses at the following locations:

- pmake: https://code.ornl.gov/99R/pmake (GPL v3)
- dwork: https://github.com/frobnitzem/dwork (GPL
  v3)
- mpi-list: Mpi-list is released in the pypi package index, and contains full documentation and functionality tests. https://github.com/frobnitzem/mpi\_list (MIT license)
- Workflow Timings: https://code.ornl.gov/99R/workflow\_timing (CC4-BY-SA)

All cases contain example use instructions, while mpi-list and dwork have more extensive tests and documentation. Usage code is provided in Fig. 1 for pmake, Fig. 2 for dwork and Fig. 3 for mpi-list. Full scripts to reproduce the results presented here are present in the workflow timings repository linked above.

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