



# ScSF: A Scheduling Simulation Framework

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**Abstract.** High-throughput and data-intensive applications are increasingly present, often composed as workflows, in the workloads of current HPC systems. At the same time, trends for future HPC systems point towards more heterogeneous systems with deeper I/O and memory hierarchies. However, current HPC schedulers are designed to support classical large tightly coupled parallel jobs over homogeneous systems. Therefore, there is an urgent need to investigate new scheduling algorithms that can manage the future workloads on HPC systems. However, there is a lack of appropriate models and frameworks to enable development, testing, and validation of new scheduling ideas.

In this paper, we present an open-source scheduler simulation framework (ScSF) that covers all the steps of scheduling research through simulation. ScSF provides capabilities for workload modeling, workload generation, system simulation, comparative workload analysis, and experiment orchestration. The simulator is designed to be run over a distributed computing infrastructure facilitating large-scale tests. We demonstrate ScSF through a case study to develop new techniques to manage scientific workflows in a batch scheduler. The evaluation consisted of 1728 experiments and equivalent to 33 years of simulated time, were run in a deployment of ScSF over a distributed infrastructure of 17 compute nodes over two months. Finally, the experimental results were analyzed using the ScSF framework to demonstrate that our technique minimizes workflow turnaround time without over-allocating resources. Finally, we discuss lessons learned from our experiences to inform future large-scale simulation studies using ScSF and other similar frameworks.

## 1 Introduction

In recent years, high-throughput and data-intensive applications are increasingly present in the workloads at HPC centers. Current trends to build larger HPC

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Source code available to download at: <http://frieda.lbl.gov/download>.

G. P. Rodrigo—Work performed while working at the Lawrence Berkeley National Lab.

systems point towards heterogeneous systems and deeper I/O and memory hierarchies. However, HPC systems and their schedulers were designed to support large communication-intensive MPI jobs run over uniform systems.

The changes in workloads and underlying hardware have resulted in an urgent need to investigate new scheduling algorithms and models. However, there is limited availability of tools to facilitate scheduling research. Currently available simulator frameworks do not capture the complexities of a production batch scheduler. Also, they are not powerful enough to simulate large experiment sets, or they do not cover all its relevant aspects, i.e., workload modeling and generation, scheduler simulation, and result analysis.

Schedulers are complex systems and their behavior is the result of the interaction of multiple mechanisms that rank and schedule jobs, while monitoring the system state. Many simulators, e.g., Alea [12], include state of art implementations of some of these mechanisms, but do not capture the interaction between the components. As a consequence, hypotheses tested on such simulators might not hold in real systems.

Scheduling behavior depends on the configurations of the scheduler and characteristics of the workload. As a consequence, the potential number of experiments needed to evaluate a scheduling improvement is high. Also, experiments have to be run for long time to be significant and have to be repeated to ensure representative results. Unfortunately, current simulation tools do not provide support to scale up and run large numbers of long experiments. Finally, workload analysis tools to correlate large scheduling result sets are not available.

In this paper, we present ScSF, a scheduling simulation framework that captures the scheduling research life-cycle. It includes a workload modeling engine, a synthetic workload generator, an instance of Slurm wrapped in a simulator, a results analyzer, and an orchestrator to coordinate experiments run over a distributed infrastructure. ScSF will be available as open source software<sup>1</sup>, enabling community extensions and user customization of modules. We also present a use case that illustrates the use of the scheduling framework for evaluating a workflow-aware scheduling algorithm. Our case study demonstrates the modeling of the workload of a peta-scale system, Edison at the National Energy Research Scientific Computing Center (NERSC). We also describe the mechanics of implementing a new scheduling algorithm in Slurm and running experiments over distributed infrastructures.

Specifically, our contributions are:

- We describe the design and implementation of scalable scheduling simulator framework (ScSF) that supports and automates workload modeling and generation, Slurm simulation, and data analysis. ScSF will be available as open source.
- We detail a case study that works as a guideline to use the framework to evaluate a workflow-aware scheduling algorithm.
- We discuss the lessons learned from running scheduling experiments at scale that will inform future research in the field.

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<sup>1</sup> Available at: <http://frieda.lbl.gov/download>.

The rest of the paper is organized as follows. In Sect. 2, we present the state of art of scheduling research tools and the previous work supporting the framework. The architecture of ScSF and the definition of its modules are presented in Sect. 3. In Sect. 4, we describe the steps to use the framework to evaluate a new scheduling algorithm. In Sect. 5, we present lessons learned while using ScSF at scale. We present our conclusions in Sect. 6.

## 2 Background

In this section, we describe the state of art and challenges in scheduling research.

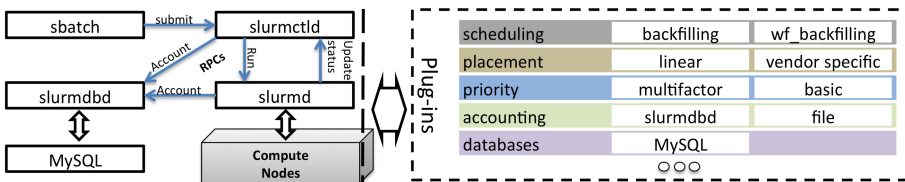
### 2.1 HPC Schedulers and Slurm

ScSF support research on HPC scheduling. The framework incorporates a full production scheduler and is modified to include new scheduling algorithms to be evaluated.

Different options were considered for the framework scheduler. Moab (scheduler) plus Torque (resource manager) [5], LSF [9], and LoadLeveler [11] are popular in HPC centers. However, their source code is not easily available which makes extensibility difficult. The Maui cluster scheduler is an open-source precursor of Moab [10]. However it has not been kept up to date to support current system needs. Slurm is one of the most popular recent workload managers in HPC. It is currently used in 5 of top 10 HPC systems [2]. It was originally developed at Lawrence Livermore National Laboratory [20], now maintained by SchedMD [2], and it is available as open source. Also, there are publicly available projects that support simulation in it [19]. Hence, our simulator framework is based on Slurm.

As illustrated in Fig. 1, Slurm is structured as a set of daemons that communicate over RPC calls:

**slurmctld** is the scheduling daemon. It contains the scheduling calculation functions and the waiting queue. It receives batch job submissions from users and distributes work across the instances of **slurmd**.



**Fig. 1.** Slurm is composed by three daemons: **slurmctld** (scheduler), **slurmd** (compute nodes management and supervision), and **slurmdbd** (accounting). A plug-in structure wraps the main functions in those daemons.

**slurmd** is the worker daemon. There can be one instance per compute node or a single instance (front-end mode) managing all nodes. It places and runs work in compute nodes and reports the resources status to `slurmctld`. The simulator uses front-end mode.

**sbatch** is a command that wraps the Slurm RPC API to submit jobs to `slurmctld`. Most commonly used by users.

Slurm has a plug-in architecture. Many of the internal functions are wrapped by C APIs loaded dynamically depending on the configuration files of Slurm (`slurmctld.conf`, `slurmd.conf`).

The Slurm simulator is a wrapper around Slurm to emulate HPC resources, emulate user's job submission, and speed up Slurm's execution. We extended previous work from the Swiss Supercomputing Center (CSCS, [19]) that is based on work by the Barcelona Supercomputing Center (BSC, [14]). Our contributions increase Slurm's speed up while maintaining determinism in the simulations, and adds workflow support.

## 2.2 HPC Workload Analysis and Generation

ScSF includes the capacity to model system workloads and generate synthetic ones accordingly. Workload modeling starts with elimination of flurries (i.e., events that are not representative and skew the model) [8]. The generator models each job variable with the empirical distribution [13], i.e., it recreates the shape of job variable distributions by constructing a histogram and CDF from the observed values.

## 2.3 Related Work

Previous work [18] proposes three main methods of scheduling algorithms research: theoretical analysis, execution on a real system, and simulation. The theoretical analysis is limited to produce boundary values on the algorithm, i.e. best and worst cases, but does not allow predicting regular performance. Also, since continuous testing of new algorithms on large real systems is not possible, simulation is the option chosen in our work.

Available simulation tools do not cover the full cycle of modeling, generation, simulation, and analysis. Also, public up-to-date simulators and workload generators are scarce. As an example, our work is based on the most recent peer reviewed work on Slurm Simulation (CSCS, [19]). We improve its synchronization to speed up its execution. For more grid-like workloads, Alea [12] is an example of a current HPC simulator. However, it does not include a production simulator in its core and does not generate workloads.

For workload modeling, function fitting and user modeling are recognized methods [7]. ScSF's workload model is based on empirical distributions [13], as it produces good enough models and does not require specific information about system users. Also, our work modeling methods are based on the experience

of our previous work on understanding workload evolution of HPC systems life cycle [15] and job heterogeneity in HPC workloads [16].

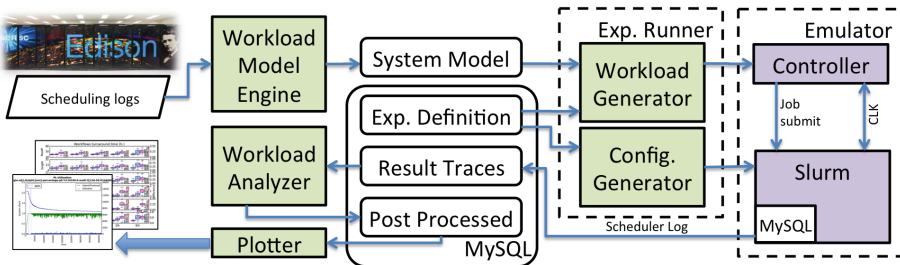
In workload generation, previous work compares close and open loop approaches [21], i.e. taking into account or not the scheduling decisions to calculate the job arrival time. ScSF is used in environments with reduced user information, which is needed to create closed-loop models. Thus, ScSF uses an open-loop workload generation model to fill and load mechanisms (Sect. 3.4) to avoid under and over job submission.

Finally, other workloads and models [6] are available, but are less representative of current HPC systems. In our work, we use workloads from Edison, a Cray XC30 supercomputer, deployed in 2013 with 133,824 cores and 357 TB of RAM.

### 3 ScSF Architecture

Figure 2 shows ScSF’s architecture. The core of ScSF is a MySQL database that stores the framework’s data and meta-data. Running experiments based on a reference system requires modeling its workload first by processing the system’s scheduling logs in the *workload model engine*. This model is used in the experiments to generate synthetic workloads with similar characteristics to the original ones.

In ScSF, the simulation process starts with the description of the experimental setup in an *experiment definition* provided by the user. The definition includes workload characteristics, scheduler configuration, and simulation time. The *experiment runner* processes experiment definitions and orchestrates experiments accordingly. First, it invokes the *workload generator* to produce a synthetic workload of similar job characteristics (size, inter arrival time) as the real ones in the reference system chosen. This workload may include specific jobs (e.g., workflows) according the experiment definition. Next, the runner invokes the simulator. The ScSF simulator is a wrapper around Slurm that increases the execution pace and emulates the HPC system and its users. The simulator sets Slurm’s configuration according to the experiment definition and emulates



**Fig. 2.** ScSF schema with green color representing components developed in this work and purple representing modified and improved components. (Color figure online)

the submission of the synthetic workload jobs. Slurm schedules the jobs over the virtual resources until the last workload job is submitted. At that moment, the simulation is considered completed.

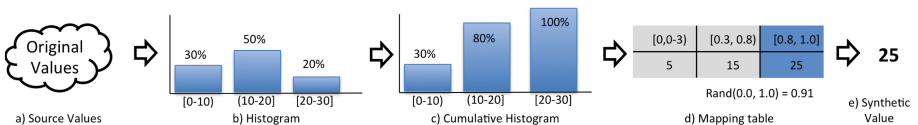
Completed simulations are processed by the *workload analyzer*. The analysis covers the characterization of jobs, workflows, and system. This module includes tools to compare experiments to differentiate the effects of scheduling behaviors on the workload.

### 3.1 Workload Model Engine

A workload model is composed of statistical data that is used to generate synthetic jobs that with characteristics similar to the original ones. The workload model engine extracts a job’s characteristics from Slurm or Moab scheduling logs including wait time, allocated CPU cores, requested wall clock time, actual runtime, inter-arrival time, and runtime accuracy ( $\frac{runtime}{requestedWallClockTime}$ ). Jobs with missing information (e.g. start time), or individual rare and very large jobs that would skew the model (e.g. system test jobs) are filtered out.

Next, the extracted values are used to produce the empirical distributions [13] of each job variable as illustrated in Fig. 3. A normalized histogram is calculated on the source values. Then, the histogram is transformed into a cumulative histogram, i.e., each bin represents the percentage of observed values that are less or equal to the upper boundary of the bin. Finally, the cumulative histogram is transformed into a table that maps probability ranges on a value. For example, in Fig. 3, bin (10 – 20] has a [0.3, 0.8) probability range as its value is 80% and its left neighboring bin’s value is 30%. The probability ranges map to the mid value of the range that they correspond to, e.g., 15 is the mid value of (10 – 20]. This model is then ready to produce values, e.g., a random number (0.91) is mapped on the table to obtain 25.

Each variable’s histogram is calculated with specific bin sizes adapted to its resolution. By default, the bin size for the request job’s wall clock time is one minute (Slurm’s resolution). The corresponding bin size for inter-arrival time is one second as that corresponds to the resolution of timestamps in the logs. Finally, for the job CPU core allocation, the bin size is the number of cores per node of the reference system, as in HPC systems node sharing is usually disabled.



**Fig. 3.** Empirical distribution constructions for job variables: calculating a cumulative histogram and transforming it into a mapping table.

### 3.2 Experiment Definition

An experiment definition outlines the conditions in an experiment process, configuring the scheduler, workload characteristics, and experiment duration. A definition is composed of a scheduler configuration file and a database entry (Table 1) that includes:

**trace\_type and subtraces:** The tag “single” identifies the experiments that are meant to be run in the simulator. A workload will be generated and run through the simulator for later analysis. The experiments with trace\_type “grouped” are definitions that list the experiments that are the different repetitions of the same experimental conditions in the “subtraces” field.

**system model:** selects which system model is to be used to produce the workload in the experiment.

**workflow\_policy:** controls presence of workflows in the workload. If set to “no”, workflows are not present. If set to “period” a workflow is submitted periodically once every workflow\_period\_s seconds. If set to “percentage”, workflows contribute workflow\_share of the workload core hours.

**Table 1.** Experiment definition fields

trace_type	“single”: regular experiment. “grouped”: experiments aggregated
subtraces	list of single experiments related to this grouped one
system	name of system to model workload after
workflow_policy	“period”: one workflow workflow_period_s. “percent”: workflow_share core hours are workflows. “no”: no workflows
manifest_list	list of workflows to appear in the workload
workflow_handling	workflows submission in workload. “single”: pilot job. “multi”: chained jobs”. “manifest”: workflow-aware job
start_date	submit time of first job valid for analysis
preload_time_s	time to prepend to the workload for stabilization
workload_duration_s	workload stops at start_date + workload_duration_s
seed	string to init random number generators

```

1 {"tasks": [
2   {"id": "SWide", "cmd": "./W.py", "cores": 480, "rtime": 360.0},
3   {"id": "SLong", "cmd": "./L.py", "cores": 48, "rtime": 1440.0,
4     "deps": ["SWide"]}]}

```

**Fig. 4.** WideLong workflow manifest in JSON format.

**manifest\_list:** List of pairs (share, workflow) defining the workflows present in the workload: e.g., {(0.4 Montage.json), (0.6 Sipt.json)} indicates that 40% of the workflows will be Montage, and 60% Sipt. The workflow field points to a JSON file specifying the structure of the workflow (e.g., Fig. 4). It includes two tasks, the first running for 6 min, allocating 480 cores (wide task); and the second running for 24 min, allocating 48 cores (long task). The SLong task requires SWide to be completed before it starts.

**workflow\_handling:** This parameter controls the method to submit workflows. The workload generator supports workflows submitted as chained jobs (*multi*), in which workflow tasks are submitted as independent jobs, expressing their relationship as job completion dependencies. Under this method, workflow tasks allocate exactly the resources they need, but intermediate job wait times might be long, increasing the turnaround time. Another approach supported is the pilot job (*single*), in which a workflow is submitted as a single job, allocating the maximum resource required within the workflow for its minimum possible runtime. The workflow tasks are run within the job, with no intermediate wait times, and thus, producing shorter turnaround times compared to chained jobs approach. However, it over-allocates resources, that are left idle at certain stages of the workflow.

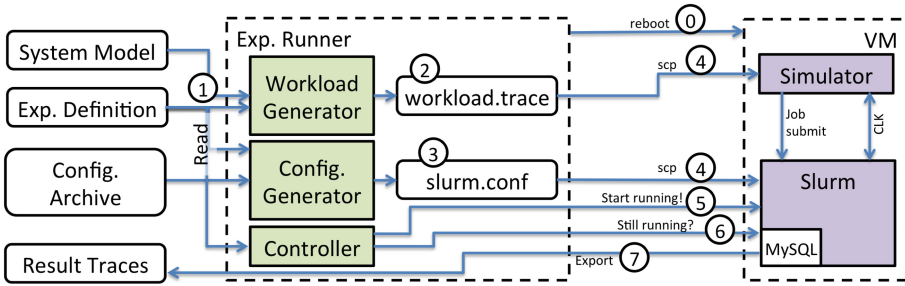
**start\_date, preload\_time\_s, and workload\_duration\_s:** defines the duration of the experiment workload. The variable start\_date sets the submit time of the first job in the analyzed section of the workload, which will span until (start\_date + workload\_duration\_s). Before the main section, a workload of preload\_time\_s seconds is prepended, to cover the cold start and stabilization of the system.

**random seed:** The random seed is an alphanumeric string that is used to initialize the random generator within the workload generator. If two experiments definitions have the same parameters, including the seed, their workloads will be identical. If two experiment definitions have the same parameters, but a different seed, their workloads will be similar in overall characteristics, but different as individual jobs (i.e. repetitions of the same experiment). In general, repetitions of the same experiment with different seeds are subtraces of a “grouped” experiment.

### 3.3 Experiment Runner

The experiment runner is an orchestration component that controls the workload generation and scheduling simulation. It invokes the workload generator and controls through SSH a virtual machine (VM) that contains a Slurm simulator instance. Figure 5 presents the experiment runner operations after being invoked with a hostname or IP of a Slurm simulator VM. First, the runner reboots the VM (step 0) to clear processes, memory, and reset the operative system state. Next, an experiment definition is retrieved from the database (step 1)





**Fig. 5.** Steps to run an experiment (numbers circled indicate order) taken by the experiment runner component. Once step seven is completed, the step sequence is re-started.

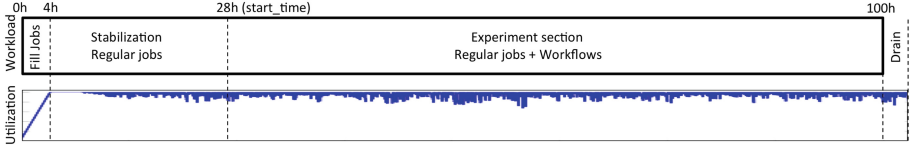
and the workload generator produces the corresponding experiment’s workload file (step 2). This file is transferred to the VM (step 4) together with the corresponding Slurm configuration files (obtained in step 3). Then, the simulation inside the VM (step 5) is started. The main part of the simulation stops after the last job of the workload is submitted. Additionally, some extra time is included in the end to avoid abrupt system termination noises in the results. The experiment runner monitors Slurm (step 6), and when it terminates, the resulting scheduler logs are extracted and inserted in the central database (step 7).

Only one experiment runner can start per simulator VM. However, multiple runners manage multiple VMs in parallel, which enables scaling such that the experiments run concurrently.

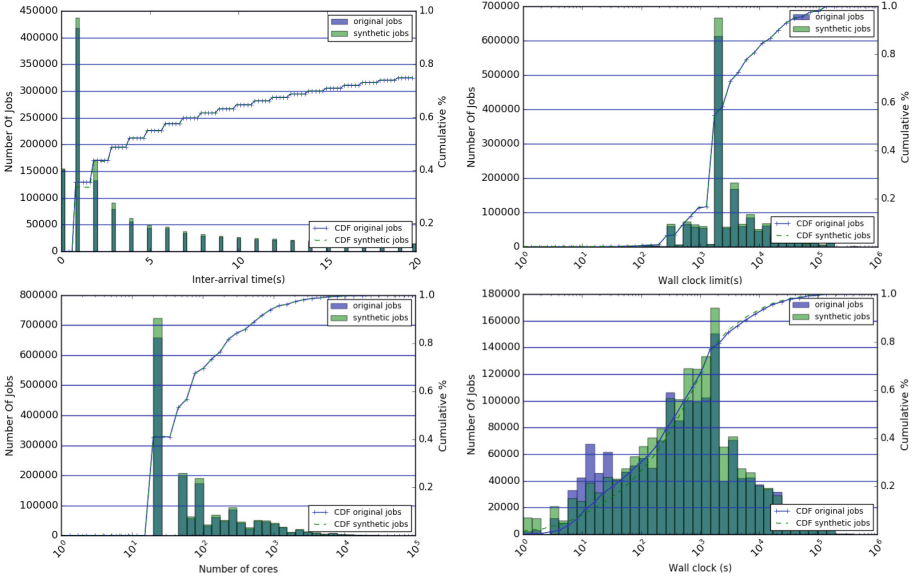
### 3.4 Workload Generation

The workload generator in ScSF produces synthetic workloads representative of real system models. The workload structure is presented in Fig. 6. All workloads start with a *fill* phase, which includes a group of jobs meant to fill the system. The fill job phase is followed by the stabilization phase, which includes 24 h of regular jobs controlled by a job-pressure mechanism to ensure that there are enough jobs to keep the system utilized. The stabilization phase captures the cold start of the system, and it is ignored in later analysis. The next stage is the experiment phase, it runs for a fixed time (72 h in the figure) and includes regular batch jobs complemented by the experiment specific jobs (in this case workflows). After the workload is completely submitted, the simulation runs for extra time (drain period, configured in the simulator) to avoid the presence of noise from the system termination.

In the rest of this section, we present all the mechanisms involved in detail.



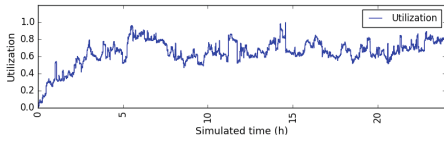
**Fig. 6.** Sections of a workload: fill, stabilization, experiment, and drain. Presented with an the associated utilization that this workload produced in the system.



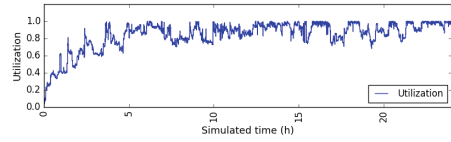
**Fig. 7.** Job characteristics in a year of Edison’s real workload (darker) vs. a year of synthetic workload (lighter). Distributions are similar.

**Job Generation:** The workload generator produces synthetic workloads according to an experiment definition. The system model is chosen among those produced by the workload model engine (Sect. 3.1). Also, the random generator is initialized with the experiment definition’s seed. The system model selected in the definition is combined with a random number generator to produce synthetic batch jobs. Finally, the workload generator also supports the inclusion of workflows according to the experiment definition (Sect. 3.2).

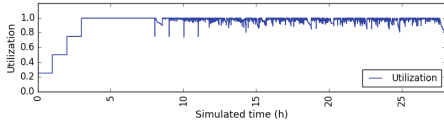
The workload generator fidelity is evaluated by modeling NERSC’s Edison and comparing one year of synthetic workload with the system jobs in 2015. The characteristics of both workloads are presented in Fig. 7, where the histogram and Cumulative distribution functions (CDFs) for inter arrival time, wall clock limit and allocated number of cores are almost identical. For runtime, there are small differences in the histogram that barely impact the CDF.



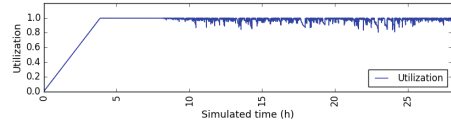
**Fig. 8.** No Job pressure mechanism, No Fill: Low utilization due not enough work.



**Fig. 9.** Job pressure 1.0, No Fill: Low utilization due to no initial filling jobs.



**Fig. 10.** Job pressure 1.0, Fill with large jobs: initial falling spikes.



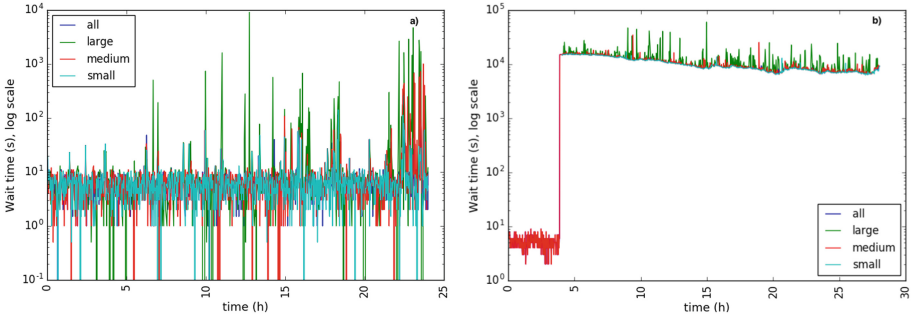
**Fig. 11.** Job pressure 1.0, Fill with small jobs: Good utilization, more stable start.

**Fill and Load Mechanisms:** Users of HPC systems submit a job load that fills the systems and creates a backlog of jobs that induces an overall wait time. The fill and load mechanisms steer the job generation to reproduce this phenomena.

The **load mechanism** ensures that the size of the backlog of jobs does not change significantly. It induces a job pressure (submitted over produced work) close to a configured value, usually 1.0. Every time a new job is added to the workload, the load mechanism calculates the current job pressure  $t$  as  $P(t) = \frac{coreHoursSubmitted}{coreHoursProduced(t)}$  where  $coreHoursProduced = t * coresInTheSystem$ . If  $P(t) < 1.0$  new jobs are generated and also inserted in the same submit time until  $P(t) \geq 1.0$ . If  $P(t) \geq 1.1$ , the submit time is maintained as reference, but the job is discarded, to avoid overflowing the system. The effect of the load mechanism is observed in Fig. 9, where the utilization raises to values close to one for the same workload parameters as in Fig. 8.

Increasing the job pressure raises system utilization but does not induce the backlog of jobs and associated overall wait time that is present in real systems. As an example, Fig. 12a presents the median wait time of the jobs submitted in every minute of the experiment using the load mechanism of Fig. 9. Here, the system is utilized but the job wait time is very short, only increasing to values of 15 min for larger jobs (over 96 core hours) at the end of the stabilization period (versus the four hours intended).

The **fill mechanism** inserts an initial job backlog equivalent to the experiment configured overall wait time. The job filling approach guarantees that they will not end at the same time or allocate too many cores. As a consequence, the scheduler is able to fill gaps left when they end. Figure 10 shows an experiment in which the fill job allocations are too big, their allocation is 33,516 cores (1/4 of the system CPU cores count). Every time a fill job ends ( $t = 8, 9, 10,$  and  $11$  h), a drop in the utilization is observed because the scheduler has to fill a large gap



**Fig. 12.** Median wait time of job's submitted in each minute. a: Job pressure 1.0, not fill mechanism, and thus no wait time baseline is present. b: Job pressure 1.0, fill mechanism configured to induce four hours of wait time baseline.

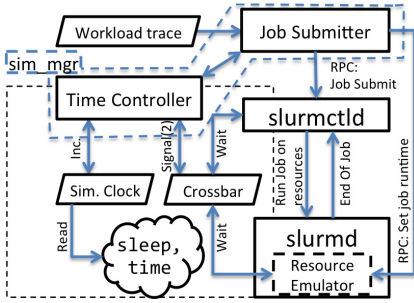
with multiple small jobs. To avoid this, the filling mechanism calculates a fill job size that induces the desired overall wait time while not producing utilization drops. Fill job size calculation is based on a fixed inter-arrival time, the capacity of the system, and the desired wait time. Figure 11 shows the utilization of a workload where fill jobs are calculated following such a method. They are submitted in 10s intervals creating the soft slope in the figure. Figure 12b shows the wait time evolution for the same workload, sustained around four hours after the fill jobs are submitted.

**Customization:** The workload generator includes classes to define user job submission patterns. Trigger classes define mechanisms to decide the insertion times pattern, such as: periodic, alarm (at one or multiple time stamps), re-programmable alarm), or random. The job pattern is set as a fixed jobs sequence, or a weighted random selection between patterns. Once a generator is integrated it is selected by setting a special string in the `workflow_policy` field of the experiment definition.

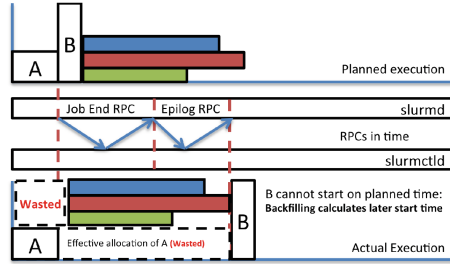
### 3.5 Slurm and the Simulator

ScSF uses Slurm version 14.3.8. as the scheduler of the framework. Also, as a real scheduler, it includes the effect and interaction of mechanisms such as priority engines, scheduling algorithms, node placement algorithms, compute nodes management, job submissions system, and scheduling accounting. Finally, Slurm includes a simulator to use it on top of an emulated version of an HPC system, submitting a trace of jobs to it, and accelerating its execution. This tool enables experimentation without requiring the use of a real HPC system.

The architecture of Slurm and its simulator is presented in Fig. 13. The Slurm daemons (`slurmctld` and `slurmd`) are wrapped by the emulator. Both daemons are dynamically linked with the `sim_func` library that adds the required functions to



**Fig. 13.** Slurm simulator architecture. Slurm system calls are replaced to speed-up execution. Scheduling is synchronized. Job submission is emulated.



**Fig. 14.** Simulated time running during RPC communications delay resource de-allocation compromising backfilling’s job planning and Job B start.

support the acceleration of Slurm’s execution. Also, slurm is compiled including a resource and job emulator. On the simulator side, the *sim\_mgr* controls the three core functions of the system: execution time acceleration, synchronization of the scheduling processes, and emulation of the job submission. These functions are described below.

**Time acceleration:** In order to accelerate the execution time, the simulator decouples the Slurm binaries from the real system time. Slurm binaries are dynamically linked with the *sim\_func* library, replacing the *time*, *sleep*, and *wait* system calls. Replaced system calls use an epoch value controlled by the *time controller*. For example, if the time controller sets the simulated time to 1485551988, any calls to *time* will return 1485551988 regardless of the system time. This reduces the wait times within Slurm i.e., if the scheduling is configured to run once every 30 simulated second, it may run once every 300 ms in “real” time.

**Scheduling and simulation synchronization:** The original simulated time pace set by CSCS produces small speed ups for large simulated systems. However, increasing the simulated time pace triggers timing problems because of the Remote Procedure Calls (RPC) in Slurm daemon communications.

Increasing the simulation pace has different negative effects. First, timeouts occur triggering multiple RPC re-transmissions degrading the performance of Slurm and the simulator. Second, job timing determinism degrades. Each time a job ends, slurm sends an RPC notification to slurmctld, and its arrival time is considered the job end time. This time is imprecise if the simulated time increases during the RPC notification propagation. As a consequence, low utilization and large job (e.g. allocating 30% of the resources) starvation occurs. Figure 14 details this effect - a large *Job<sub>B</sub>* is to be executed after *Job<sub>A</sub>*. However, *Job<sub>A</sub>* resources are not considered free until two sequential RPC calls are completed (end of job

and epilogue), lowering the utilization as they are not producing work. The later resource release also disables  $Job_B$  from starting but does not stop the jobs that programmed are to start after  $Job_B$ . As the process repeats, the utilization loss accumulates and  $Job_B$  is delayed indefinitely.

The *time\_controller* component of the *sim\_mgr* was modified to control a synchronization crossbar among the Slurm functions that are relevant to the scheduling timing. This solves the described synchronization problems by controlling the simulation time and avoiding its increase while RPC calls are traveling between the Slurm daemons.

**Job submission and simulation:** The job submission component of the *sim\_mgr* emulates the submission of jobs to *slurmctld* following the workload trace of the simulation. Before submitting each job, it communicates the actual runtime (different from the requested one) to the resource emulator in *slurmd*.

The daemon, *slurmctld*, notifies *slurmd* of the scheduling of a job. The emulator uses the notification arrival time and job runtime (received from *sim\_mgr*) to calculate the job end time. When the job end time is reached, the emulator forces *slurmd* to communicate that the job has ended to *slurmctld*. This process emulates the job execution and resource allocation.

### 3.6 Workload Analyzer

ScSF includes analysis tools to extract relevant information across repetitions of the same experiment or to plot and compare results from multiple experimental conditions.

**Value Extraction and Analysis:** Simulation results are processed by the workload analyzer. The jobs in the fill, stabilization, and drain phases (Fig. 6) are discarded to extract (1) for all jobs: wait time, runtime, requested runtime, user accuracy (estimating the runtime), allocated CPU cores, turnaround time, and slowdown grouped by jobs sizes. (2) for all and by type of workflow: wait time, runtime, turnaround time, and stretch factor. (3) overall: median job wait time and mean utilization for each minute of the experiment.

The module performs different analyses for different data types. Percentile and histograms analyze the distribution and trend of the jobs' and workflows' variables. Integrated utilization (i.e.,  $\text{coreHoursProduced}/\text{coreHoursExecuted}$ ) measures the impact of the scheduling behavior on the system usage.

Finally, customized analysis modules can be added to the analysis pipeline.

**Repetitions and Comparisons:** Experiments are repeated with different random seeds to ensure that observed phenomena are not isolated occurrences. The workload analysis module analyzes all the repetitions together, merging the results to ease later analysis. Also, experiments might be grouped if they differ only in one experimental condition. The analysis module studies these groups together to analyze the effect of that experimental condition on the system.

For instance, some experiments are identical except for the workflow submission method, which affects the number of workflows that get executed in each experiment. The module calculates compared workflow turnaround times correcting any possible results skew derived from the difference in the number of executed workflows.

**Result Analysis and Plotting:** Analysis results are stored in the database to allow review of visualization using the *plotter* component. This component includes tools to plot histograms (Fig. 7), box plots, and bar charts on the median of job's and workflow's variables for one or multiple experiments (Fig. 17). It also includes tools to plot the per minute utilization (Figs. 8, 9, 10 and 11) and per minute median job wait time in an experiment (Figs. 12a and b), which allows us to observe dynamic effects within the simulation. Finally, it also include tools to extract and compare utilization values from multiple experiments.

## 4 ScSF Case Study

In this section, we describe a case study that demonstrates the use of ScSF. The case study implements and evaluates a workflow-aware scheduling algorithm [17]. In particular, we model a real HPC system, and implement a new algorithm in the Slurm simulator. Also, we detail a distributed deployment of ScSF for our evaluation and present examples of the results to illustrate the scalability of the ScSF framework.

### 4.1 Tuning the Model

Experiments to evaluate a scheduling algorithm require workload and system models that are representative. NERSC's Edison is chosen as the reference system. Its workload is modeled by processing almost four years of its jobs. In ScSF, a Slurm configuration is defined to imitate Edison's scheduler behavior, including - Edison's resource definition (number of nodes and hardware configuration) FCFS, backfilling with a depth of 50 jobs once every 30s, and a multi-factor priority model that takes into account age (older-higher) and job geometry (smaller-higher). The workload tuning is completed by running a set of experiments to explore different job pressure and filling configurations to induce a stable four hour wait time baseline (observed in Edison).

### 4.2 Implementing a Workflow Scheduling Algorithm in Slurm

As presented in Sect. 3.2, workflows are run as pilot jobs (i.e., single job over-allocation resources) or chained jobs (i.e., task jobs linked by dependencies supporting long turnaround times). However, the workflow-aware scheduling [17] is a third method that enables per job task resource allocation, while minimizing the intermediate wait times.

The algorithm integration required us to modify Slurm’s jobs submission system, and include some actions on the job queue before and after scheduling happens. First, `sbatch`, Slurm’s job submission RPC, and the internal `job_record` data structure are extended to support the inclusion workflow manifests in jobs. This enables workflow-aware jobs to be present as pilot jobs attaching a workflow description (manifest).

Second, queue transformation actions are inserted before and after FCFS and backfilling act on it. Before they act, workflow jobs are transformed into task jobs but keeping the original job priority. When the scheduling is completed, original workflow jobs are restored. As a consequence, workflow task jobs are scheduled individually, but, as they share the same priority, the workflow intermediate wait times are minimized.

### 4.3 Experiment Setup

The workflow-aware scheduling approach is evaluated by comparing its effect on workflow turnaround time and system utilization with the pilot and chained job ones. Three versions (one per approach) of experiments are created to compare the performance of the three approaches under different conditions.

Table 2 shows the three sets the experiments created. Workflows in *set0*, exhibit different structures to study their interaction with different approaches. *Set1* studies the effect of the approaches on isolated workflows and includes four real (Montage, Sipt, Cybershake, FloodPlain [4]) and two synthetic workflows submitted with different intervals (0, 1/12h, 1/6h, 1/h, 2/h, 6/h). *Set2* studies the effect of the approaches on systems increasing dominated by workflows. It includes the same workflows as *set1* submitted with different workflow shares (1%, 5%, 10%, 25%, 50%, 75%, 100%). In total, they sum 1728 experiments equivalent to 33 years of simulated time.

Experiments are created and stored using a Python class that is initialized with all the experiment parameters. The manifest files for the synthetic workflows are created manually following the framework’s manifest JSON format. Real workflow manifests are created using a workflow generator from the Pegasus project [4] that captures the characteristics of science workflows. ScSF includes a tool to transform the output of the workflow generator into the expected JSON format.

**Table 2.** Summary of experiments run in ScSF.

Set	Wf. Submit	#Wfs.	Wf. Pres.	#Pres.	Sim. t.	#Reps	#Exps	Agg. Sim. t.
Set0	aware/single/multi	18	Period	1 per wf.	7d	6	324	2268d
Set1	aware/single/multi	6	Period	6	7d	6	648	4536d
Set2	aware/single/multi	6	Share	7	7d	6	756	5292d



### 4.4 Running Experiments at Scale

We run 1728 individual experiments that sum 33 years of simulated time. Estimating an average speedup of  $10\times$ , experiment simulation would require more than three years of real time. In order to reduce the real time required to complete this work, simulation are parallelized to increase throughput.

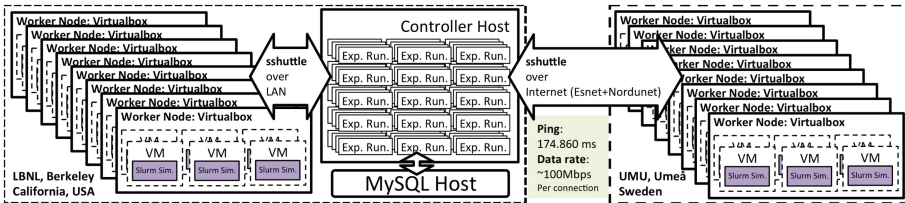
As presented in Sect. 3, the minimum experiment worker unit is composed by an instance of the *experiment runner* component and a VM containing the Slurm simulator. As shown in Fig. 15, parallelization is achieved by running multiple worker units concurrently. To configure the infrastructure, Virtualbox’s hypervisor is deployed on six compute nodes at the Lawrence Berkeley National Lab (LBNL) and 17 compute nodes at Umeå University (UMU). 161 Slurm Simulator VMs are deployed across the two sites. Each VM allocates two cores, four GB of RAM, and 20 GB of storage. Each compute node has different configurations and thus, the number of VMs per host and their performance is not uniform, e.g., some compute nodes only host two VMs, and some host 15.

All the experiment runners run in a single compute node at LBNL (Ubuntu, 12 cores  $\times$  2.8 GHz, 36 GB RAM). However, VMs are not exposed directly through their host NIC and required access from the control node over *sshuttle* [3], a VPN over ssh software that does not required installation on the destination host. Even if both sites are distant, the network is not a significant source of problem since the connection between UMU and LBNL traverses two high performance research networks, Nordunet (Sweden) and ESnet (EU and USA). Latency is relatively low (170–200 ms), data-rate is high (firewall capped  $\approx 100$  Mbits/s per TCP flow), and stability consistent.

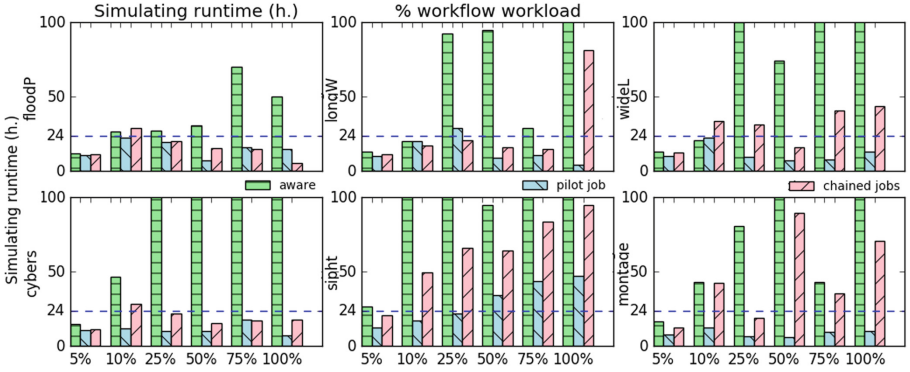
### 4.5 Experiment Performance

The experiments wall clock time is characterized as a function of the experiment setup to understand the factors driving simulation speed-up. Figure 16 shows the experiments median runtime of one experiment set, grouped by scheduling method, workflow type, and workflow presence.

For the same simulated time, simulations run longer under the chained job and workflow-aware approaches compared to pilot job. Also, for the chained



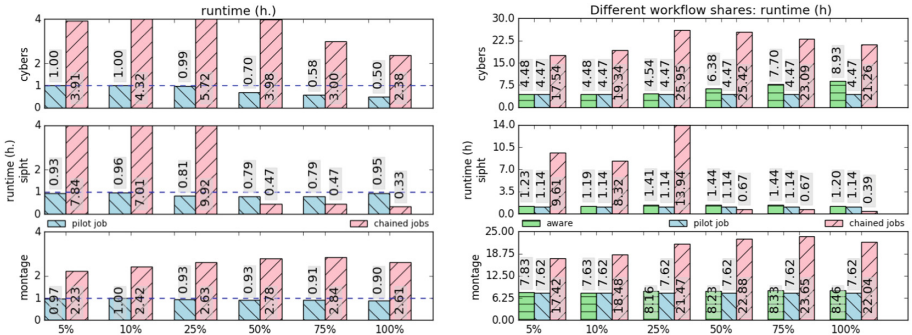
**Fig. 15.** Schema of the distributed execution environment: VMs containing the Slurm Simulator are distributed in hosts at LBNL and UMU. Each VM is controlled by an instance of the experiment runner in the controller host at LBNL.



**Fig. 16.** Median wall clock time for a set of simulation. More complex workloads (more workflows, large workflows) present longer times. Pilot job approach presents shorter times. Simulation time is 168 h (7 days).

job and aware approaches, experiments run longer time if more workflows are present, or the workflows include more task jobs. As individual experiments are analyzed, longer runtimes, and thus smaller speed-ups, appear to be related to longer runtime of the scheduling passes because of higher numbers of jobs in the waiting queue.

In summary, simulations containing numbers of jobs similar to real system workloads present median runtimes between 10 to 12 h for 7 days (168 h) of simulated time, or  $15\times$  speedup. Speed-up degrades as experiments become more complex. Speed-ups under 1 are observed for experiments whose large job count would be hard to manage for a production scheduler (e.g., Montage-75%). The limiting factor of the simulations speed-up is the scheduling runtime, which, in this case study, depends on the number of jobs in the waiting queue.



**Fig. 17.** Comparison of median workflow runtime on different experimental conditions as speed-up (left), and absolute numbers (right). Data of workflows in 108 experiments.

## 4.6 Analyzing at Scale

The analysis of the presented use case required synthesis of the results of 1278 experiments into meaningful, understandable metrics. The tools described in Sect. 3.6 supported this task.

As an example, Fig. 17 condenses the results of 324 experiments (six repetitions per experiment setting): median workflow runtime speed up (left) and value (right) observed for Cybershake, Sipht, and Montage, for different workflow shares and scheduling approaches. Results show that chained job workflows support much longer runtime in all cases, while aware and pilot jobs workflows show shorter (than chained job workflows) but similar runtimes to each other.

## 5 Discussion

The initial design goal of ScSF was functionality, not scale, and its first deployment included four worker VMs. As the number experiments and simulation time expanded for our case study (33 years), the resource pool size had to be increased (161 VMs and 24 physical hosts), even expanding to resources in distributed locations.

**Loss-less experiment restart is needed:** As the framework runs longer and on more nodes, the probability for node reboots becomes higher. In the months of experiments our resources required rebooting due to power cuts, hypervisor failures, VM freezes, and system updates (e.g. we had to update the whole cluster to patch the Dirty Cow exploit [1]).

Our goal in ScSF has been to keep the design light-weight and easily portable. Thus, rebooting a worker host means that work in the VMs are lost. Also, if the controller host is rebooted, all the experiment runners are stopped and the work in the entire cluster is lost. For some of the longest experiments, the amount of work lost accounts in days of real time. In the future, we need to consider the trade-offs and ScSF should include support graceful pause and restart so resource reboots do not imply loss of work. This would be provided by a control mechanism to pause-restart worker VMs. Also, the experiment runner functionality should be hosted in the worker VM to be paused with the VM, unaffected by any reboot.

**Loaded systems network fail:** In our experiments, surges of experiment failures appeared occasionally. Multiple VMs would become temporarily unresponsive to ssh connections when their hypervisor was heavily loaded. Subsequently, the experiment runner would fail to connect to the VM, and the experiment was considered failed. Thus, saturated resources are unreliable. All runner-VM communications were hardened, adding re-trials, which reduced the failure rate significantly.

**Monitoring is important:** Many types of failures impact experiments, such as simulator or Slurm bugs, communication problems, resource saturation in the VMs, or hypervisor configuration issues. Failures are expected, but early version

of ScSF lacked the tools and information to quickly diagnose the cause of the problems. Monitoring should register metadata that allows quick diagnosis of problems. As a consequence, the logging levels were increased and a mechanism to retrieve Slurm crash debug files was added.

**The system is as weak as its weakest link:** All ScSF's data and metadata are stored in a MySQL database hosted in the controller host. In a first experiment run, at 80% of completed experiments the hard disk containing the database crashed, and all experiment data was lost that included two months of work. Currently, data is subject to periodic backups and the database is replicated.

## 6 Conclusions

We present ScSF, a scheduling simulation framework which provides tools to support all the steps of the scheduling research cycle - modeling, generation, simulation, and result analysis. ScSF is scalable, it is deployed over distributed resources to run and manage multiple concurrent simulations and provides tools to synthesize results over large experiment sets. The framework produces representative results by relying on Slurm, which captures the behavior of real system schedulers. ScSF is also modular and might be extended by the community to generate customized workloads or calculate new analyses metrics over the results. Finally, we improved the Slurm simulator which now achieves up to  $15\times$  simulation over real time speed-ups while preserving its determinism and experiment repeatability.

This work provides a foundation for future scheduling research. ScSF will be released as open source, enabling scheduling scientists to concentrate their effort on designing scheduling techniques and evaluating them in the framework. Also, we share our experience of using ScSF to design a workflow scheduling algorithm and evaluating it through the simulation of a large experiment set. Our case study demonstrates that the framework is capable of simulating 33 years of real system time in less than two months over a distributed infrastructure.

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