RLScheduler: Learn to Schedule HPC Batch Jobs Using Deep Reinforcement Learning

A Preprint

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Abstract

We present RLScheduler, a deep reinforcement learning based job scheduler for scheduling independent batch jobs in high-performance computing (HPC) environment. From knowing nothing about scheduling at beginning, RLScheduler is able to autonomously learn how to effectively schedule HPC batch jobs, targeting a given optimization goal. This is achieved by deep reinforcement learning with the help of specially designed neural network structures and various optimizations to stabilize and accelerate the learning. Our results show that RLScheduler can outperform existing heuristic scheduling algorithms, including a manually fine-tuned machine learning-based scheduler on the same workload. More importantly, we show that RLScheduler does not blindly over-fit the given workload to achieve such optimization, instead, it learns general rules for scheduling batch jobs which can be further applied to different workloads and systems to achieve similarly optimized performance. We also demonstrate that RLScheduler is capable of adjusting itself along with changing goals and workloads, making it an attractive solution for the future autonomous HPC management.

1 Introduction

Although jobs in high-performance computing (HPC) platforms are increasingly diverse today, most of them are still fixed, rigid, and non-preemptable batch jobs in practice [1]. Here, fixed means each job will require a fixed amount of computation resources; rigid means the jobs will not negotiate about their required resources, and will not run if the requested resources are not fulfilled; non-preemptable means once the jobs start, they will run until either finished, failed, or got killed, without being suspended and resumed. In HPC, these batch jobs are submitted to a centralized job scheduler, which picks jobs to run once encounters a scheduling point, such as new job arrived or occupied resources released (due to job completions, failures, or terminations). Most of the HPC job schedulers are work conserving, i.e., it will always try to make a scheduling attempt if possible. Typically, system administrators will configure the job schedulers to optimize certain system metrics, such as resource utilization, average job wait time, or makespan, etc. Although it sounds simple, finding an optimal batch job scheduler towards a certain goal has been a long-studied, classic NP-hard problem [2].

Numerous heuristic HPC batch job schedulers have been studied [3–9]. Most of them leverage a heuristic priority function to schedule jobs. The heuristic priority function takes the characteristics of jobs (e.g., resource requirements, waiting time) and potentially the states of the system (e.g., the available resources) as inputs and output a priority value for each job. Then, the scheduler can use it to order all the jobs and schedule the top ones. For example, the well-known shortest job first (SJF) algorithm sorts jobs based on their estimated execution time (e.g., the maximal execution time specified in job scripts), trying to reduce the average job waiting time by scheduling shorter jobs first [10]. More realistic job management systems, such as Slurm [11], TORQUE [12], or PBS [13], allow combining multiple factors into consideration in their priority functions [3]. System administrators can configure the weight of each factor to optimize the system.
Although the tremendous amount of research on scheduling has deepened our understanding about priority function and its potential consequences towards an optimization goal, heuristically tweaking the scheduler’s priority function to achieve a certain system optimization goal is still a challenging task for even the most experienced HPC system administrators due to the complexity of the scheduling problem itself. For example, a recent study [4] show that four priority functions that combine jobs’ characteristics in an unexpected non-linear way can actually produce extremely high-quality scheduling decisions comparing with existing methods. Such a non-linear combination is infeasible for system administrators to identify manually. In fact, not only manually changing the priority functions might lead to suboptimal results, it may further lead to unexpected consequences that are hard to reason and potentially risky.

We believe that it would be very promising that if the job scheduler can autonomously learn how to schedule batch jobs to achieve a given optimization goal, such as minimizing job waiting time, maximizing system utilization, or a combination of them. In this way, the administrators can focus more on designing appropriate goals for their systems and let the scheduler itself figure out how to make the scheduling decisions to best achieve that goal.

Following such an idea, in this study, we propose RLScheduler, an HPC job scheduler which leverages deep reinforcement learning techniques [14, 15] to autonomously learn how to schedule HPC batch jobs. We show that, from scratch, a well-designed deep reinforcement learning agent (e.g., our RLScheduler) can effectively learn how to make good scheduling decisions on a given system, even compared with the manually fine-tuned machine learning-based scheduler. More importantly, we further show that our RLScheduler does not blindly over-fit a given system or workload to achieve that optimization, instead, it learns general scheduling rules that can be directly applied to other workloads to achieve similarly optimized performance. We also show RLScheduler is capable of adjusting itself along with changing goals and workloads, making it attractive in real systems. In summary, we make the following key contributions in this study:

- We show that deep reinforcement learning agents can effectively learn how to schedule HPC batch jobs. The learned rules are generally applicable to different workloads and systems.
- We propose a set of design choices and optimizations in RLScheduler to stabilize and accelerate deep reinforcement learning for HPC job scheduling tasks.
- We show that RLScheduler is capable of adapting to different optimization goals, making it attractive for autonomous HPC job management.

The remainder of this paper is organized as follows: In Section II we introduce HPC batch job scheduling problem itself, the reinforcement learning basis, and the motivations and challenges behind this study. In Section III we present the proposed RLScheduler and its key designs and optimizations. We present the main results (i.e. the RLScheduler and its performances) in Section IV, and the conclusions and future work in Section V.

2 Background and Challenges

2.1 HPC Batch Job Scheduling

In this study, we limit our scope in a homogeneous high-performance computing environment and focus on scheduling independent batch jobs. These assumptions do not suggest the deep reinforcement learning techniques are limited to this scenario. Mao et. al. showed that deep reinforcement learning can be used in scheduling dependent Spark tasks [16]. To build the basis of this study, in this subsection, we describe several key aspects of the HPC job scheduling problem.

[Job Features] HPC batch job has multiple features can be seen in job script, such as user id, group id, requested nodes, maximal execution time, and the submitted queue, etc. A complete feature list of job can be seen in the Standard Workload Format (SWF) [17]. Although all these job features can be potentially useful for making scheduling decisions, in this study, we focus on a subset of them (as listed below), mainly for making fair comparisons with other schedulers. The deep learning model used in RLScheduler is actually in a better position to leverage such extensive information [18]. We plan to investigate how extra information can further improve RLScheduler in the future work.

- The id of a job \(id\).
- The submission time of a job \(s_t\).
- The requested computing nodes of a job \(n_c\).
- The requested execution time of a job \(r_t\).
Note that, modern HPC may provision the system into multiple queues, so jobs might be submitted to different queues and scheduled separately. In this study, we focus on the conventional batch queue, where most batch jobs are submitted to.

[Scheduling and Backfilling] In HPC, all jobs arrive in a centralized, global job queue (batch queue) and wait there for scheduling. Once a job is picked, the system will try to provision its requested resources. If success, the job will start to run. If fail, the system will wait until the requested resources are fulfilled [11]. While waiting, backfilling will be activated to improve the resource utilization [6]. It looks for jobs that will not affect the planned execution of the picked job and schedules them to run. In this way, without delaying the picked job, the scheduler can improve the overall resource utilization. Nowadays, backfilling is by default enabled in most HPC batch job schedulers. We also enable it in this study.

[Scheduling Goal] In practice, there could be many diverse goals that system administrators or users want to optimize via scheduling. It is even possible to consider multiple goals at the same time. Defining an appropriate goal itself is a challenging task and out of the scope of this paper.

In this study, to show the effectiveness of RLScheduler, we heavily compare RLScheduler with one of the state-of-the-art machine learning-based job scheduler [4]. To make a fair comparison, we set our optimization goal the same as its. But, we do show that RLScheduler can perform the same on a different goal in the evaluation section. For the majority part of this paper, we use a simple but widely used metric called bounded slowdown [19] as our goal to optimize:

\[ \text{bsld} = \max \left( \frac{w_t + r_t}{\max(r_t, \tau)}, 1 \right) \]  

\( w_t \) is the time that a job waits in the job queue; \( \tau \) is a constant, with a typical value of 10s to prevent small tasks from having excessively large slowdown values. For a set of jobs, the goal is to minimize the average bounded slowdown.

[Markov Decision Process] To leverage reinforcement learning, we check the Markov property of batch job scheduling task. In fact, we can safely model most HPC job scheduling as a finite Markov Decision Process (MDP) [20], as each scheduling decision is made based on the states of current pending jobs, current running jobs, and availability of HPC system, independent of the previous states and actions (i.e., the Markov property). The actual mapping is quite straightforward: the state includes the current waiting jobs, running jobs, and the availability of resources; the action is the job scheduled; the transition is the changes on the waiting jobs, running jobs, and resources availability once a job was scheduled to run; and the reward is the measurement of optimization goal we cared about. In this sense, scheduling HPC batch jobs turns into solving a finite MDP problem, and can be solved using reinforcement learning methods.

2.2 Deep Reinforcement Learning

Reinforcement learning (RL) is a type of machine learning technique that enables an agent to autonomously learn in an interactive environment by trial and error using feedback from its own actions and experiences [14, 15].

Fig. 1 shows its general framework. At each time step \( t \), the agent observes some state \( S_t \), and decides to choose action \( A_t \). Then the action will change the environment from \( S_t \) to \( S_{t+1} \) and the agent receives reward \( R_{t+1} \). For most of the cases, the agent does not have a prior knowledge of which state the environment would transition to or what the reward may be. During training, the agent can observe them. The goal of learning is to maximize the expected cumulative discounted reward collected from the environment: \( E[\sum_{t=0}^{\infty} \gamma^t r_t] \), where \( \gamma \in (0, 1] \) is a discounting factor on future rewards.

The agent picks actions based on a policy, defined as a probability distribution \( \pi : \pi(s, a) \rightarrow [0, 1] \). It simply means the probability of taking action \( a \) at state \( s \). Since the state spaces could be enormous, it is impossible to have an
accurate $\pi$ distribution. Instead, we can use deep neural networks to estimate the distribution. In this way, the agent will take similar actions for "close-by" states [18]. The reinforcement learning using deep neural networks to model the policy of agent is then called Deep Reinforcement Learning (DRL).

There are multiple ways to train the DRL agent [15]. In this study, we heavily leveraged the policy gradient method [21–23]. It learns by performing gradient-descent directly on the policy parameters ($\theta$). The essential idea of such method is to let the agent collect a set of trajectories $\tau = (s_0, a_0, s_1, a_1, \ldots)$ using its current policy ($\pi_\theta$) first. Here $s_0$ is the initial state of the system and should be randomly generated from a start-state distribution; then $a_t$ and $s_{t+1}$ are just the consequence of picking the next action and the new state. All the actions are picked using the same policy $\pi_\theta$ and the trajectory stops when the whole interaction is done. For each $\tau$, we can collect cumulative rewards based on all the interactions between agent and environment: $R(\tau) = \sum_{t=0}^{\infty} \gamma^t r_t$. Then the goal is to select a policy ($\pi_\theta$) which maximizes expected return when the agent acts according to it for a set of sampled trajectories:

$$J(\pi_\theta) = E_{\tau \sim \pi_\theta}[R(\tau)]$$

This can be done by updating the $\theta$ based along direction of the $J(\pi_\theta)$’s gradient: $\nabla_\theta J(\pi_\theta)$. More details about policy gradient can be seen at [15].

2.3 Motivations and Challenges

The very recent successes of deep reinforcement learning (DRL) in problems such as playing Go [24] and complicated video games [25] inspires us to leverage it in HPC batch job scheduling. Comparing with traditional schedulers, DRL-based one does have several advantages. It learns by just interacting with the environment, freeing the HPC system administrators from tediously trying different priority functions to build their fine-tuned schedulers. The deep model is complex and should be able to recognize more subtle differences of the system states and produce high-quality scheduling decisions [18]. Also, DRL learns via continuously interacting with the environment [15], making the scheduler able to adapt to the changing goals and workloads without human intervention.

However, applying deep reinforcement learning in HPC batch job scheduling is non-trivial. First, HPC batch job scheduling actually has much larger state space and action space even comparing with the classic DRL solvable tasks such as playing Go [24]. In typical HPC environments, there could be thousands of jobs waiting for scheduling and over ten thousand of compute nodes available. This indicates a large search space for the reinforcement learning agent to explore, potentially making the learning impractically long.

Second, unlike Go, the HPC environments are highly dynamic. Its behaviors not only dependent on the agent’s actions but also dependent on the upcoming job sequences. The high variance of arriving job sequences can easily confuse the reinforcement learning algorithms. For example, if in job sequence A, jobs only arrived after the previous one finished, then the average slowdown will be optimal no matter which scheduling algorithm was used. On the other hand, if a job sequence has all jobs arrived all together, then no matter which scheduling algorithm was used, the average bounded slowdown will be large. If the agent happens to sample a lot of the first case, then it will consider its own scheduling policy good, even it is actually worse. To eliminate this effect, we have to make the training independent from the actual job arriving sequence to stabilize the training.

Last but not the least, deep neural networks utilized in deep reinforcement learning will require fixed numerical vectors as the inputs, but the inputs to the HPC job scheduler are an uncertain number of waiting jobs. It is then necessary to find a way to map HPC job scheduling states to fixed vectors usable to neural networks, while at the same time, minimize the negative effects on the training.

In the next section, we will introduce the detailed design and implementation of RLScheduler, and how we solve previous challenges in RLScheduler.

3 Design and Implementation

Fig. 2 shows the overall architecture of RLScheduler, which is structured based on the general framework of deep reinforcement learning. At each time step, the Agent (3.1), which is constructed by two neural networks (i.e., policy and value networks), observes a State (3.3) from the environment SchedGym (3.2) and makes decision on the next Action (3.4). The action will be applied to the environment again and change its state to a new one. The agent also receives reward (3.5) from the environment after making the action. After this, another iteration will start as the new state will be feed to the agent again. The agent learns from its past actions and the rewards it collects cumulatively. The iteration stops when the environment reaches a final state. When stopped, the agent collects a trajectory and can use it to update its current policy ($\pi_\theta$) using policy gradient method. We will discuss each of these components in more detail in the next several subsections.
3.1 RLScheduler Agent

The core of deep reinforcement learning is its agent (i.e., the deep neural networks), which is trained to accurately model the system state and generate the correct actions. In RLScheduler, we introduce two designs to facilitate the training: 1) inspired by the priority function concept, we design a kernel-based network structure optimized for job scheduling; 2) leveraging the actor-critic model, we use a value network to reduce the high variance of HPC job scheduling task [15].

3.1.1 Policy network structure

RLScheduler agent contains two neural networks: policy network and value network. The policy network represents the policy ($\pi$). It takes current pending jobs as input and outputs the probability of scheduling each of them. We will discuss the role of value network in the next subsection.

Fig. 3 shows the detailed structure of policy network. This kernel-based structure is inspired by the fact that most existing heuristic job schedulers are essentially using a priority function which takes job features as inputs and outputs its priority value to schedule. So, we set a window, which will take one job each time as the input to the same kernel network. The kernel is simply a multiple layer perceptron (MLP) [26] network. It outputs a single value for each job. The outputs of different jobs are combined and feed to Softmax to generate the final probability. In RLScheduler, we are able to control the parameter size of policy network less than 5.
1,000. We will compare our network with naively using CNN and MLP and demonstrate its advantages in the later evaluations section.

### 3.1.2 Value network and variance reduction

We use value network in RLScheduler to further stabilize and accelerate the training. As discussed in 2.3, the random job sequences in HPC increases the variance of the environment and may confuse the agent. The value network is used to solve this issue. It outputs a single adjustment value for each state to eliminate the effects of variant job sequences.

Specifically, the value network is a 3-layer MLP network. But, different from policy network, it takes all the job vectors together (flatted and sorted using FCFS) as the input and outputs a single float value. This float value will be trained based on the actual rewards collected from all previous scheduling for the same state. In this way, this output value can be intuitively considered as the expected reward \((c_{exp})\) or baseline reward of a state according to the agent’s previous policies. It denotes how best the agent can do on a given state historically. With this value, during training, RLScheduler will not use the direct rewards \((r)\) it collects from environment to train the policy network, instead, it will use \((r - c_{exp})\) as the actual reward for training. Such a reward will much less be affected by the random job sequence, as it is not directly comparing rewards collected from different job sequence scheduling, instead, it is comparing the improvements of current policy over historical policies on the same job sequence, which significantly reduces the variances.

### 3.2 SchedGym Environment

The reinforcement learning agent needs an enormous number of interactions to learn, which is not practical in a running HPC system. A more realistic way to train DRL-based job scheduler from a cold start is to collect the job workloads from the real system periodically and train the agent in a simulated environment using the collected real-world workloads. To do this, we implemented a simulated HPC environment, named SchedGym based on the OpenAI Gym toolkit to facilitate the training. OpenAI Gym is a generic platform for developing and comparing reinforcement learning algorithms [28].

SchedGym simulates a homogeneous HPC environment to virtually run batch jobs (by just moving forward the timestamp instead of actually running them). All the batch jobs are created based on the actual job traces collected from real systems (SWF workload archive [17]), following exactly the same order and submission time. The actual runtime of a job will be used by SchedGym to move forward the timestamp to simulate the resources releasing.

Whenever a scheduling point arrives, such as a new job arrived or occupied resources released, SchedGym will query the scheduler for a scheduling action, and act based on the action returned. It is possible the scheduled jobs can not run because the available resources are not enough. In this case, SchedGym will wait until enough resources are released. While waiting, SchedGym will backfill jobs that will not affect the previously picked jobs to run. Once finishing scheduling (i.e., no jobs are waiting or running), SchedGym resets itself to a random initial state (starting from a random timestamp in the job trace), schedules another sequence of jobs (the length of the sequence is configurable) again to generate another trajectory. We implemented SchedGym using discrete-event simulation. More details can be found in the source repo [29].

In HPC, batch jobs may arrive continuously, preventing SchedGym to reach the final state to generate the training trajectory. To avoid this, in RLScheduler, we leveraged the batch training strategy [16]. Each time, SchedGym chooses a batch of jobs to train. As long as all the jobs in this batch have been scheduled, SchedGym will reach a final state and generate the trajectory. The batch size is tunable. But it should not be too small, as the RLScheduler agent will try to over-fit the short job sequences and learn exceptionally good scheduling rules that only work on the same short job sequences from the same trace. Large batch size can avoid such an issue as the number of possible job sequences increases exponentially as batch size increases, preventing the over-fitting. Our results in the evaluation section also prove the generality when training with 512 batch size. The trained model can be applied to different job sequence sizes and different workloads. Since larger batch size also increases the training time and memory pressure, we set the default batch size to be 512 in RLScheduler.

### 3.3 RLScheduler Observable State

State is the input of deep reinforcement learning agent. In RLScheduler, we incorporate two important info in the state to help make the scheduling decisions: 1) pending jobs info, and 2) available resource info.

More specifically, RLScheduler arranges state as a vector of job vectors, as the colored rectangles shown in Fig. 3. Each vector represents a job, consist of three attributes from the job itself (job arriving time \(n_r\), request computation resources of the job \(n_c\), requested runtime of the job \(r_t\)) and one attribute from the cluster (available resources \(avail_t\)).
We noticed that, directly using avail requires RL Scheduler to learn the relationship between available resources (avail) and requested resources (nc) for each job implicitly. So, to make it more straightforward for the agent, we actually use at = availt − nc to abstract the availability. This value simply means the expected available resources if the job was scheduled to run. In this way, each job vector is [st, nc, rt, at], and the whole state is a vector of these vectors.

3.3.1 Observation Padding and Cut-off

In the real system, the number of pending jobs changes, hence the size of the vector should also change accordingly. However, deep neural network only takes a fixed-size vector as inputs. To solve this, we set the observable system state to be a fixed size (MAX_OBSV_SIZE). If there are fewer pending jobs, we pad the vector with all 0s job vector; if there are more pending jobs, we cut-off them selectively. The number of observable jobs is a configurable training parameter. We set it to 128 in RLScheduler by default, as many HPC job management systems, such as Slurm, also limit the number of pending jobs to the same order of magnitude [30].

3.3.2 Suggested Candidates

Since only a fixed number of jobs are observable to the agent, we certainly hope the best scheduling candidates are among them. So, when cut-off the pending jobs, we leverage heuristic scheduling algorithms to generate suggested candidates and avoid cutting them. Specifically, we leverage SJF and FCFS to sort the pending jobs separately and choose jobs from both the sorted list in a round-robin way. These suggested candidates should have better chances to be the final scheduled job. In our evaluations, we will show how suggestions can help the performance.

3.3.3 Sorting

Once determining the observable jobs, the next thing is to place them into the vector, which will be represented to the agent. Since our policy network is order insensitive, in RLScheduler, we will just randomly shuffle all the jobs before feeding them to the RLScheduler agent. Our results in the evaluation section also show sorting order does not affect the training of our RLScheduler.

3.4 RLScheduler Scheduling Action

Action is what reinforcement learning agents take based on their observations. In RLScheduler, the action is as simple as just picking up one job in the observable jobs and attempting to schedule it. One problem, though, is how to handle the padded, all 0s jobs. These padded jobs do not actually exist and should not be handled by the SchedGym environment. To solve such an issue, RLScheduler agent will mask illegal jobs when the policy network outputs the probability of scheduling each job. In this way, RLScheduler will never output illegal action to SchedGym environment.

3.5 RLScheduler Reward

Reward is the feedback that reinforcement learning agents collect from the environment. Its goal is to maximize cumulative rewards. Reward is the key for the agents to learn in the expected direction. In this study, we set the goal as minimizing average bounded slowdown (bsld_avg), which simply means that the deep reinforcement learning agent should strive for maximizing −bsld_avg. Here, the average is calculated based on all jobs in a job sequence:

\[ bsld_{avg} = \frac{\sum_{j \in seq} bsld(j)}{|seq|} \]

Scheduling a job sequence involves multiple actions made by the RLScheduler agent. In reinforcement learning, each time the agent takes an action, it expects to receive a reward. But, at this time, we can not calculate the average yet. In RLScheduler, we return a reward of 0 when the entire job sequence has not been scheduled yet. Only after the whole sequence was scheduled, the average slowdown for all jobs in the job sequence will be calculated and returned as a reward to the agent as ‘−bsld_avg’.

4 Evaluation

We implemented RLScheduler using Tensorflow [31]. For the training process, we leveraged Proximal Policy Optimization (PPO) algorithm derived from OpenAI Spinning Up library [23]. Our code is open-source on Github [29].
4.1 Evaluation Setup

In the evaluation, we utilized both synthetic workloads and real-world workloads and compared different scheduling algorithms. The real-world workloads are from SWF archive [17], as shown in the top portion of Table 1. The synthetic workload (Lublin-256) is generated based on real-world workloads distribution [32]. We chose this particular job trace because it has been widely used in many batch job scheduling studies, including the state-of-the-art machine learning-based batch job schedulers [4]. We aim to directly compare with the state-of-the-art algorithms on the same job trace. Also, unless explicitly specify, we used the same RLScheduler agent trained on the Lublin-256 dataset in most of the following evaluations.

| Name        | Date | Mons | CPUs |
|-------------|------|------|------|
| CTC-SP2     | 1996 | 11   | 338  |
| SDSC-SP2    | 1998 | 24   | 128  |
| SDSC-Blue   | 2000 | 32   | 1,152|
| HPC2N       | 2002 | 42   | 240  |
| ANL Intrepid| 2009 | 8    | 163,840|
| Lublin-256  | -    | -    | 256  |

Table 1: List of Workloads

In our evaluations, we compared RLScheduler with several baseline heuristic job scheduling algorithms, shown in Table 2. Here, FCFS schedules jobs in the same order as they were submitted (i.e., using $s_t$). SJF schedules jobs based on how long the job will run (i.e., using $r_t$). Note that, the job execution time by default is based on the maximal execution time specified in the job script. Most of real-world job traces have such value. If not (such as the synthetic workloads), we will use the actual execution time instead, which will make SJF perform impractically good. WFP3 and UNICEP belong to the family of schedulers that combines multiple factors [3]. They favor jobs with smaller runtime, fewer resource requirements, and longer waiting time, representing the expert knowledge of tweaking the priority functions. Scheduler F1 is from [4], representing the state-of-the-art machine learning-based scheduling algorithms for minimizing the average bounded slowdown of jobs. Table 2 shows all their detailed score functions.

| Name    | Function                                      |
|---------|-----------------------------------------------|
| FCFS    | $score(t) = s_t$                              |
| SJF     | $score(t) = r_t$                              |
| WFP3    | $score(t) = -(w_t/r_t)^3 \cdot n_t$           |
| UNICEP  | $score(t) = -w_t/(\log_2(n_t) \cdot r_t)$     |
| F1      | $score(t) = \log_{10}(r_t) \cdot n_t + 870 \cdot \log_{10}(s_t)$ |

Table 2: List of heuristic scheduling functions

4.2 RLScheduler Training Evaluation

In this subsection, we show how RLScheduler was trained and how the designs and optimizations we introduced in RLScheduler help accelerate and stabilize the training.

4.2.1 The importance of network structure

RLScheduler has a window based neural network structure in policy network to help with HPC batch job scheduling task. Fig. 4(a) shows the effectiveness of such a new network structure. It plots the training process of RLScheduler with different neural networks (i.e., our own, CNN, and MLP) on the same workload (Lublin-256) using the same configurations. From this plot, we can have two observations regarding the training processes with different network structures. First, our RLScheduler converges much faster (in the first 0.2 million interactions) and converges to a larger value ($-60$). Second, RLSchedulerCNN and RLSchedulerMLP converge as well but much slower and to a much smaller value ($-90$). These results clearly show the benefits and importance of the new network. Here, both RLSchedulerCNN and RLSchedulerMLP take all the job vectors together (flatted and sorted) as inputs and outputs a probability vector. This represents a naive way of using deep neural networks in job scheduling tasks. We used basic CNN and 3-layer MLP in this test. The number of parameters for both cases is around 100K.
4.2.2 The importance of suggested candidates

In RL Scheduler, to handle the mismatch between possibly long job queue in HPC and the fixed size input of neural networks, we cut off the original job queue to a fixed size based on the suggestions from two simple heuristic algorithms SJF and FCFS. Fig. 4(b) shows the difference between RL Scheduler with and without suggested candidates. We can see that RL Scheduler converged at almost the same speed in both cases. But, with suggested candidates, RL Scheduler keeps achieving better performance (around +10) during the training. Note that, to conduct this evaluation, we reduced the observable jobs for RL Scheduler from the default 128 to 16, simply because the 128 fixed queue is too large that our training dataset can not fill the fixed queue in most of the time and hence barely show any difference.

4.2.3 The insensitivity to job order

Once choosing the observable jobs, the next step is to determine the order of these jobs that RL Scheduler can observe. Such an order might make a difference during the training if the neural network is not built properly. In our test, we noticed that the order significantly changes the behaviors of RL Scheduler CNN and RL Scheduler MLP, occasionally leading to results that do not converge. However, using the designed networks, RL Scheduler is insensitive to the order of the observable jobs anymore as the training curve shown in Figure 4(c). This clearly reveals the advantages and robustness of RL Scheduler.

4.3 RL Scheduler Performance Evaluation

In this subsection, we report and compare how RL Scheduler actually performs on scheduling job sequences selected from synthetic and real-world job traces.

4.3.1 Scheduling synthetic trace

We first show how RL Scheduler performs when it is used to schedule the same trace that it was trained on (i.e., Lublin-256). The training set and testing set take 70% and 30% of the dataset respectively. Fig. 5 shows the results of different scheduling algorithms scheduling 10 randomly picked sequence of jobs from the synthetic job trace Lublin-256. From these results, we can see that, in all cases, the RL Scheduler clearly outperforms other algorithms, including the state-of-the-art F1 scheduler. Please note that this is actually an ideal case for RL Scheduler. But, it is also the ideal case for the machine learning-based algorithms (e.g., F1) as they were also trained based on the same workload [4]. One may argue that the good performance of RL Scheduler may come from over-fitting the training workload. We will show its generality in the next evaluations.

4.3.2 Scheduling real-world traces

We further evaluated how RL Scheduler performs in various real-world traces which it has never seen before. In this evaluation, we compared RL Scheduler (the same one trained on Lublin-256) with other heuristic schedulers on 5 real-world traces (shown in Table 1) and a new synthetic trace as shown in Fig. 6. From the results, we can see that, among all the real-world data traces, RL Scheduler (RL) clearly outperforms manually designed heuristic schedulers, such as FCFS, WFP, UNI, and SJF. In addition, it also performs better or at least comparable with the machine learning-based F1 algorithm. This clearly shows the generality of what RL Scheduler learns. One thing worths noting is the results
Figure 5: The performance of RLScheduler (RL) and other scheduler algorithms on Lublin-256. The evaluated RLScheduler was trained on the same job trace (on the training dataset). We picked 10 samples and each sample contains 2,048 jobs to cover roughly 1 week’s jobs. Here, y-axis is the average bounded slowdown calculated after scheduling the whole job sequence; the orange line in the box is the mean of all samples.

Figure 6: The performance of RLScheduler (RL) and other schedulers on various workloads. Note the evaluated RLScheduler was trained on Lublin-256, not on these job traces. 10 random job sequences were picked, each contains 2,048 jobs.

on a new synthetic dataset (i.e., Lublin-256-New). The dataset was generated intentionally different from the original Lublin-256 (with smaller job arrival interval and smaller average job size). In this case, both F1 and our RLScheduler which were trained on Lublin-256, becomes less effective as expected, while SJF performs well due to the heavily loaded small jobs. However, different from F1, given new workloads, RLScheduler will be able to learn, adjust its own scheduler policy, and eventually achieve better performance. We already show how RLScheduler can learn from scratch in previous evaluation (e.g., Fig 4).
4.3.3 Visualizing what RLScheduler learns

To further explain what RLScheduler actually learns and why it can perform well in various workloads and systems, we visualized the scheduling of sequence of jobs using RLScheduler and SJF in Fig. 7. Here, we first used a simple job sequence to explain what RLScheduler learns, then visualized a more complex and realistic case, which shows similar patterns. Note that, we used the RLScheduler agent trained on Lublin-256 here.

In the simple scheduling case (Fig. 7(a)), we can see RLScheduler performs better than SJF in terms of both average bsld and overall makespan. If look at the scheduling decision for each job in more detail, we can see one obvious difference between RLScheduler and SJF: Task-1 was scheduled much later in RLScheduler, but much earlier in SJF. Among all jobs in the sample, Task-1 is actually a relatively short task, but requires more resources. SJF blindly prioritize such a short job, hoping to reduce the average job waiting time. However, because it takes more resources, scheduling it too early actually delays all other jobs, leading to a worse result. While, on the other hand, RLScheduler considers the needed resources of a job as an important factor and delays scheduling Task-1 until it is more appropriate. In Fig. 7(b), we show the more complex case with 512 jobs scheduled. Although the visualization looks complicated, we can again see a similar pattern that jobs needing longer execution time but fewer resources are scheduler earlier in RLScheduler to increase the system utilization and improve the bounded slowdown.

![Visualization of scheduling process](image)

Figure 7: The scheduling process of RLScheduler and SJF on two different job sequences. For both figures (a and b), the upper part shows how the scheduling actually happened: x-axis shows the timeline, the y-axis shows the servers taken by each job. The lower part of each figure shows the calculated bounded slowdown (bsld) for each job when it got scheduled. The average values are also shown in the top right corner. For the sample job sequence (a), there are 16 servers in total. When scheduling starts, the first two jobs are running and all other jobs are pending. For the real job sequence (b), the job sequence was randomly selected from Lublin-256, which has 256 servers in total.

4.4 RLScheduler Towards A Different Goal

A major advantage of RLScheduler is that it can autonomously learn how to make optimized scheduling decisions once given a specific goal. This will free system administrators from tedious tasks such as adjusting scheduler parameters.

To show this, in this evaluation, we changed our optimization goal from minimizing the average bounded slowdown to minimize the average waiting time and tested whether RLScheduler can still effectively learn how to schedule jobs towards this new goal. It is very simple to make such a modification in RLScheduler, we just changed the reward.
Figure 8: The training progress of RLScheduler on Lublin-256 towards a different goal (minimize average job wait time). Here, x-axis shows the total interactions between the agent and SchedGym environment. y-axis shows the performance of the agent, referring to $-\text{average wait time}$.

value calculation to be $-\text{average wait time}$ and trained the model again. Due to the space limitation, we only briefly discuss its training progress and scheduling performance below.

Fig. 8 plots the training progress of RLScheduler on Lublin-256 data traces towards the new goal, we can see that although the y-axis has changed significantly as the goal is changed, the training of RLScheduler still converges fast within the first 0.5 million interactions with the environments.

Figure 9: The performance of RLScheduler (RL) vs other schedulers on sampled job traces.

Fig. 9 further plots the actual performance of using newly trained RLScheduler on the Lublin-256 data-trace. The setting is similar to the results shown in Fig. 5. From this plot, we can see that RLScheduler outperforms other scheduling algorithms in this new metric, which proves that RLScheduler can autonomously learn effective scheduling policy towards a different goal.

5 Related Work

HPC batch job scheduling has been a long-time research topic. Numerous studies have been done in this domain [3–5, 5–9]. The taken approaches are pretty widely ranged: from classic policies such as First Come First Served (FCFS) or Shortest Job First (SJF) to smarter and more complex policies such as WFP3 and UNICEF [3]; from linear programming [9, 33] to generic algorithms [34, 35] and even neural networks [7, 8]. RLScheduler is clearly different from most of these existing studies as it explores the new deep reinforcement learning-based approach, aiming to be both optimized and adaptable.
Recently, several studies also started to leverage deep reinforcement learning in resource allocation and job scheduling in a distributed environment, such as DeepRM [36, 37], and Decima [16]. Although they used similar DRL methods as RLScheduler, these studies are not designed for scheduling HPC jobs, which are fixed, rigid, and non-preemptable. These differences lead to different reinforcement learning designs and optimizations in RLScheduler, detailed in Section 3.

Currently, the state-of-the-art HPC batch job scheduling comes from [4]. It used brute force simulations to generate a large number of data samples, each of which shows the best scheduling decision given a random job sequence. Then, applying machine learning methods on these data samples to build scheduling functions that can best-fit these samples. RLScheduler is different from this study as it uses a totally different learning strategy (reinforcement learning v.s supervised learning). Comparing with them, RLScheduler achieves similar or even better performance, and most importantly, is adaptive and autonomous.

6 Conclusion and Future Plan

In this study, we present RLScheduler, a deep reinforcement learning-based job scheduler, which autonomously learns how to schedule HPC batch jobs. We show that RLScheduler can learn high quality and general scheduling rules given an optimization goal. In addition, it can adjust itself towards different goals and workloads effectively. We believe reinforcement learning-based methods are attractive for managing a much more complex HPC system in the future, and RLScheduler would be the first step towards that goal. For the next step, we plan to further investigate more realistic HPC job scheduling settings, such as leveraging more job features and targeting more complex optimization goals. In addition, we also plan to integrate RLScheduler into real HPC cluster management tools such as Slurm.

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