Design and Performance Characterization of RADICAL-Pilot on Titan

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Abstract. Many extreme scale scientific applications have workloads comprised of a large number of individual high-performance tasks. The Pilot abstraction decouples workload specification, resource management, and task execution via job placeholders and late-binding. As such, suitable implementations of the Pilot abstraction can support the collective execution of large number of tasks on supercomputers. We introduce RADICAL-Pilot (RP) as a portable, modular and extensible Python-based Pilot system. We describe RP’s design, architecture and implementation. We characterize its performance and show its ability to scalably execute workloads comprised of thousands of MPI tasks on Titan—a DOE leadership class facility. Specifically, we investigate RP’s weak (strong) scaling properties up to 131K (65K) cores and 4096 (16384) 32 core tasks. RADICAL-Pilot can be used stand-alone, as well as integrated with other tools as a runtime system.

1 Introduction

Supercomputers have been designed to support applications comprised of mostly monolithic, single-job workloads. Many existing scientific applications have workloads comprised of multiple heterogeneous tasks. A computational task is a generalized term for a stand-alone process that has well defined input, output, termination criteria, and dedicated resources. A task can be used to represent an independent simulation or data processing analysis, running on one or more nodes of a high-performance computing machine, that may or not use MPI. The number of such applications account for an increasing fraction of high-performance computing utilization \cite{1,2}.

Further, supercomputers are typically operated to maximize overall system utilization, which entails static resource partitioning across jobs and users. Thus, there is a tension between the resource requirements of non-traditional applications comprised of many smaller tasks, and the capabilities of the traditional HPC system software as well as their usage policies. Whether these applications directly access supercomputers, or use workflow systems, they could benefit from better execution and resource management on HPC resources \cite{3}. The increasing number of systems \cite{2} that address this problem is testimony to its importance.
Pilot systems address two apparently contradictory requirements: accessing HPC resources via their centralized schedulers while letting applications independently schedule tasks on the acquired portion of resources. By implementing multi-level scheduling and late-binding, Pilot systems lower task scheduling overhead, enable higher task execution throughput, and allow greater control over the resources acquired to execute workloads. As such, Pilot systems provide a promising starting point to ease the tension between the resource requirements of workloads comprised of multiple tasks and the capabilities of the traditional HPC system software.

We introduce RADICAL-Pilot (RP), a Pilot system that implements the pilot paradigm as outlined in Ref. [4]. RP is implemented in Python and provides a well-defined API and usage modes. Although RP is a vehicle for research in scalable computing, it also supports production-grade science. Currently, it is being used by applications drawn from diverse domains, ranging from earth sciences and biomolecular sciences to high-energy physics. RP directly supports their use of supercomputers or it can be used as a runtime system by third-party workflow or workload management systems [5–11].

RP is not a workflow system and does not provide workflow or workload management capabilities itself. In 2017, RP was used to support more than 100M core-hours on US DOE, NSF resources (Blue Waters and XSEDE), and European supercomputers (Archer and SuperMUC). In 2018, RP is the core runtime system for three DOE INCITE and an NSF PRAC award consuming an estimated lower bound of 250M core hours on several HPC machines, including Titan, Blue Waters (NCSA), and XSEDE resources (e.g., Stampede).

A primary contribution of this paper is the investigation and fine-grained characterization of the performance and scaling of RP to execute workloads comprised of thousands of MPI tasks on Titan, managed at the Oak Ridge Leadership Computing Facility. Consequently, we are able to localize the overheads to specific components (sub-systems) of RP and thereby optimize its performance. Specifically, we investigate RP’s weak (strong) scaling properties up to 131K (65K) cores and 4096 (16384) 32 core tasks.

Although RP works on multiple platforms, we focus our experiments on Titan—a DOE leadership class facility, as it currently offers the highest degree of concurrent execution in the USA for open/academic research (approximately 300K CPU cores). On Titan, we optimized RP to overcome existing bottlenecks, so that both the performance and scalability of RP is determined by system software limits. Specifically, we show that the launch rate of tasks is dominated by an overhead arising from the use of OpenMPI Runtime Environment (ORTE) of OpenMPI. We also observe failures at the ORTE layer when utilizing more than 131K cores.

In Section 2, we discuss existing pilot-systems and highlight the distinctive capabilities of RP. Section 3 discusses the design and architecture of RP. Section 4 describes the core experiments and results of the paper.
2 Related Work

Ref. [4] established a distinction between the Pilot paradigm and the Pilot abstraction. The Pilot paradigm refers to the execution of a workload via multi-entity and multi-stage scheduling on resource placeholders. The Pilot abstraction is associated with logical components and functionalities of software systems. By design, the Pilot paradigm enables the handling of multiple types of tasks, regardless of their size and duration. There is an apparent gap in the space of Pilot system implementations, as they have not exploited the full generality of the Pilot paradigm.

Ref. [4] presents around twenty systems that have implemented core Pilot abstraction functionality (i.e., Pilot systems) since 1995. Most of these systems are tailored to specific workloads, resources, interfaces, or development models. Most Pilot systems have been implemented to optimize the throughput of single-core (or single-node), short-lived, uncoupled tasks [4]. For example, HTCondor with Glidein on OSG [12] is one of the most widely used Pilot systems but serves mostly single core workloads; or the Pilot systems developed for the LHC communities which execute millions of jobs a week [13] specialize on supporting LHC workloads and, in most cases, specific resources like those of WLCG.

Away from distributed high-throughput pilots, the light-weight execution framework called Falkon represents an early stand-alone Pilot system for HPC environments [14]. It implements concurrency at multiple levels (e.g., dispatching, scheduling, etc.) and was optimized for single core applications. Falkon’s design allows it to achieve great performance by leaving out non-essential features like, for example, the support for multi-node tasks such as MPI [15].

The Pilot abstraction has also been implemented by various workflow management systems: for example, Pegasus [16] uses Glidein via providers like Corral [17]; Makeflow [18] and FireWorks [19] enable users to manually start workers on HPC resources via master/worker tools called Work Queue [20] or LaunchPad [19]; and Swift [21] can use Falkon [14] and Coasters [22] as Pilot systems. In most cases, the logical components that implement the Pilot abstraction are not stand-alone, nor is the functionality isolated in these workflow management systems. This can limit portability and re-usability.

JETS [23] is a middleware component that provides high performance support for many-parallel-task computing. It is designed for running short-duration MPI tasks, down to the order of seconds. Workloads can be codified in the Swift scripting language, and can be executed either by stand-alone workers (via MPICH2 [24]) or by pilots managed by Coasters. Given JETS focus on scalability of tasks with duration in the range of seconds, resource utilization is reduced at larger number of nodes or processes per node due to the increased relative delay in starting tasks across larger fractions of allocated resources.

There are systems that implement a specific set of the Pilot abstraction’s functionality to fulfill specific needs. For example, Pegasus-MPI-Cluster (PMC) [25], which is an MPI-based Master/Worker framework that can be used in combination with Pegasus. This enables Pegasus to run large-scale workflows of small tasks on HPC resources, but the tasks are limited to single-node execu-
tion. In addition, there is a dependency on `fork()/exec()` on the compute node which certain HPC resources do not support (e.g. IBM BG/Q).

The Pilot paradigm has proven sufficiently useful for certain types of workloads that resource manager systems have begun to include pilot capabilities either as separate tooling, or as part of their implementation. For example, CRAM [26] is a tool developed specifically to execute static ensembles of MPI tasks on HPC resources. Developed for Sequoia, an IBM BG/Q system at LLNL, CRAM parallelizes the execution of an application with many input parameters by statically bundling it into a single MPI executable.

Flux is described as a next-generation Scalable Resource and Job Management Software (RJMS) for HPC centers that focuses on a new paradigm of resource and job management. Within this new paradigm, Flux allows resource allocation to be dynamic (i.e., dynamic workloads), a key design principle of the Pilot paradigm. This results in jobs having the ability to scale up to a maximum requested during execution. Unfortunately, Flux is limited only to those HPC resources that use it as their RJMS. Further, as of the writing of this paper, Flux is still on an Alpha release, not suitable for production use.

As illustrated above, there has been various implementations of Pilot systems in the past, but such systems tend to be limited to certain resources, specialized to specific types of workloads, or a combination of tools is needed to implement the Pilot abstraction’s functionality. Consequently, many of these systems are limited in their ability, if able at all, to support the execution of workloads comprised of multi-core and multi-node tasks of many minutes to hour-long duration on HPC machines. We address these limitations via RADICAL-Pilot (RP), a Pilot system designed to natively and effectively support these types of workloads at scale.

3 Design of RADICAL-Pilot

RADICAL-Pilot (RP) is a runtime system designed to execute multiple types of scientific workloads on pilots instantiated on one or more resources. RP enables the description of generic workloads with one or more scalar, MPI, OpenMP, multi-process, and multi-threading tasks. These tasks can be executed on CPUs, GPUs and other accelerators, on the same pilot or across multiple pilots. We focus the discussion of design and architecture for HPC platforms.

RP implements two main abstractions: Pilot and Compute Unit (CU). Pilots and CUs abstract away specificities of resources and workloads, making it possible to schedule workloads either concurrently or sequentially on resource placeholders. Pilots are placeholders for computing resources, where resources are represented independent from architecture and topological details. CUs are units of work (i.e., tasks), specified as an application executable alongside its resource and execution environment requirements.

As a runtime system, RP offers an API to describe both pilots and CUs, alongside classes and methods to manage acquisition of resources, scheduling of CUs on those resources, and the staging of input and output files. Reporting
capabilities update the user about ongoing executions and profiling capabilities enable detailed postmortem analysis of workload executions and runtime behavior.

3.1 Architecture and Implementation

RP is a distributed system with four modules: PilotManager, UnitManager, Agent and DB (Fig. 1, purple boxes). Modules can execute locally or remotely, communicating and coordinating over TCP/IP, and enabling multiple deployment scenarios. For example, users can run PilotManager and UnitManager locally, and distribute DB and one or more instances of Agent on remote computing infrastructures. Alternatively, users can run all RP components on a remote resource.

PilotManager, UnitManager and Agent have multiple components, isolated into separate processes. Some of the module’s components are used only in specific deployment scenarios, depending on both workload requirements and resource capabilities. Components are stateless and some of them can be instantiated concurrently to enable RP to manage multiple pilots and units at the same time. This enables scaling of throughput and tolerance to failing components. Concurrent components are coordinated via a dedicated communication mesh, which introduces runtime and infrastructure-specific overheads, but improves overall scalability of the system and lowers component complexity. Components can have different implementations, configuration files can tailor RP toward specific resources types, workloads, or scaling requirements.

PilotManager has a main component called ‘Launcher’ (Fig. 1). The Launcher uses resource configuration files to define the number, placement, and properties of the Agent’s components of each Pilot. Currently, configuration files are made available for essentially all US NSF and DOE production resources as well as Beowulf variants, but users can provide new files or alter existing configuration parameters at runtime, both for a single pilot or a whole RP session.

Agent has four main components: one Stager for input and output data, Scheduler and Executor (Fig. 1). Multiple instances of the Stager and Executor components can coexist in a single Agent. Depending on the architecture of the resource, the Agent’s components can individually be placed on cluster head nodes, MOM nodes, compute nodes, virtual machines, or any combination thereof. ZeroMQ communication bridges connect the Agent components, creating a network to support the transitions of the units through components.

Once instantiated, each Agent’s Scheduler gathers information from the resource manager (RM) retrieving the number of CPUs (cores) and GPUs held by the pilot on which the Agent is running and how those cores are partitioned.
across nodes. Currently, the Scheduler acquires information from physical or virtual Linux machines and the following RMs: TORQUE, PBS Pro, SLURM, SGE, LSF, LoadLeveler, and Cray CCM.

Depending on requirements, the Agent’s Scheduler assigns cores and GPUs from one or more nodes to each unit. For example, cores on a single node are assigned to multithreaded units while, cores on topologically close nodes are assigned to MPI units to minimize communication overheads. Two scheduling algorithms are currently supported: “Continuous” for nodes organized as a continuum, and “Torus” for nodes organized in an n-dimensional torus, as found, for example, on IBM BG/Q.

The Agent’s Scheduler passes the units on to one of the Agent’s Executors, which use resource configuration parameters to derive the launching command of each unit. Currently, RP supports the following launching methods: MPIRUN, MPIEXEC, APRUN, CCMRUN, RUNJOB, DPLACE, IBRUN, ORTE, RSH, SSH, POE, and FORK. Among these, ORTE (Open RunTime Environment) enables scaling pilots on leadership-class machines beyond the limited amount of concurrent process allowed by methods like APRUN, MPIEXEC or MPIRUN.

Once the launching command is determined and further qualified depending on the unit parameters and on the characteristics of the execution environment, the Agent’s Executors will execute those commands to spawn the application processes. Different spawning mechanisms are available: “Popen” (based on Python), “Shell” (based on /bin/sh, and “ORTELIB” (based on the libopen-rte API, bound to Python via CFFI). Executors monitor the execution of the units, collect exit codes, and communicate the freed cores to the Agent’s Scheduler.

3.2 Execution Model

Workloads and pilots are described via the Pilot API and passed to the RP runtime system (Fig. 1). The PilotManager submits pilots on one or more resources via the SAGA API (Fig. 1). The SAGA API implements an adapter for each supported resource type, exposing uniform methods for job and data management. Once a pilot becomes active on a resource, it bootstraps the Agent module (Fig. 1).

The UnitManager schedules each unit to an Agent (Fig. 1) via a queue on a MongoDB instance. This instance is used as the RP DB module to communicate the workload between UnitManagers and Agents. Each Agent pulls its units from the DB module (Fig. 1) schedules each unit on the Executor when the required amount of computing resources are available (e.g., number of cores or GPUs). The Executor sets up the unit’s execution environment and then spawns the unit for execution.
Once a unit returns from its execution, the Executor communicates to the Scheduler that resources have been freed. Scheduling loop can then proceed until no units are left to execute. Once all the workload has been executed, the runtime system is terminated to avoid inefficiencies in the use of resource allocation. Multiple workloads can be executed within the time boundaries during which resource are available, determined by constraints, for example, walltime, preemption, or cost.

When required, the input data of a unit are either pushed to the Agent or pulled from the Agent, depending on data locality and sharing requirements. Similarly, the output data of the unit are staged out by the Agent and Unit-Manager to a specified destination, e.g., a filesystem accessible by the Agent or the user workstation. Both input and output staging are optional, depending on the requirements of the units. The actual file transfers are enacted via SAGA, and currently support (gsi)-scp, (gsi)-sftp, Globus Online, and of course local filesystem operations.

### 3.3 Profiling

The distributed, modular, and concurrent design of RP introduces complexities with both usability and performance overheads. The performance overheads of RP’s design require experimental characterization as they depend on the properties of both the workloads and the resources used for the execution. The execution overheads introduced at resource level are particularly relevant as they affect the execution of every unit, independent of whether the workload is divided in stages, or bounded by task dependences. The overheads introduced by bootstrapping the components of the Agent, scheduling the units, and launching them contribute to the overall time to completion of the workload, and also affect overall resource utilization.

The characterization of RP performance requires dedicated capabilities. We developed a profiler to enable postmortem performance analysis. The RP profiler collects up to 200 unique events across all module components. Each event contains a timestamp; an event identifier; component process and thread IDs; IDs of pilots and units involved. Each time stamp is recorded asynchronously to disk so as to minimize the overhead of the profiling. The resulting profiles provide complete, timestamped traces for most operations on any of the entities managed by RP: pilots, units and input/output files.

Profiling adds a certain overhead, and results as presented in this publication all include that overhead. By using buffered I/O and small data structures we can keep the overhead manageable: a typical run from the scaling experiments has pilot runtime of $1045.5 \pm 29.4s$ without profiling, and of $1069.2 \pm 49.5s$ when profiling is turned on. Profiling thus increases the runtime of about $2.5\%$, and also slightly increases the noise of the measurements.

A challenge in analyzing profiles from distributed systems such as RP is clock synchronization. Our post-mortem analysis toolchain called RADICAL-Analytics (RA) synchronizes profile timestamps via NTP synchronization points. It also performs consistency checks on the profile data, and runs different
time series analysis to provide detailed insight into RPs runtime behavior. We use RA in Section 4 to characterize RP’s performance.

4 Performance Characterization

In this section, we focus on characterizing the performance of RP when executing workloads requiring an ensemble of up to 16,000 independent MPI tasks. Such workloads are representative of several scientific domains, and pose unprecedented computational challenges due to the number of tasks, even though the size of individual MPI tasks might be modest. The scalable execution of such workloads requires leadership-class HPC machines, which are typically designed and often optimized to support the execution of single, very large MPI jobs, making it challenging to coordinate the concurrent and sequential execution of thousands of modest sized MPI tasks.

The Pilot abstraction addresses these challenges by decoupling the acquisition from the assignment of resources: once resources are acquired via a single large pilot job, a pilot Agent is used to schedule and manage the execution of tasks on those resources. We characterize the scaling and performance of RP in terms of mean time to execution (TTX) of a workload and the computing resource utilization (RU).

4.1 Experiments Design

The execution of workloads requires the interplay of all RP components and their supporting infrastructure. Nonetheless, as seen in §3, Figures 1-2, RP reduces every workload down to the execution of a set of compute units on an Agent. The Agent retrieves units individually or in bulk and executes them on its resources. As such, the characterization of TTX and RU depends on how each Agent component performs.

As explained in §1 and §3, the Pilot abstraction and the RP Agent enable the execution of tasks both concurrently and sequentially. Above a certain number of tasks, the workload cannot be executed with full concurrency, even on the largest HPC machines currently available. In this situation, sequential “batched” execution incur overheads determined by the systems and resources used to manage the execution.

Our experiments are designed to measure the overhead that the Agent, third-party libraries, and the resources add to the execution of the workload. Overhead captures the time spent either waiting for the workload’s computation to start, or performing operations other than those required by the workload. This overhead determines a partial utilization of the available computing time for executing the workload and, therefore, a certain degree of inefficiency of its execution. We investigate its growth with increasing number of units and cores.

We designed two experiments to measure the overhead of the Agent when executing the workloads described in §1. The first experiment measures the weak
scaling properties of the Agent by maintaining a constant ratio of units to resources. The second experiment measures the strong scaling of the Agent measured by fixing the number of units while varying resources.

The experiments use a workload comprised of tasks involving the MD simulations of the bovine pancreatic trypsin inhibitor (BPTI), a globular protein of 20521 atoms when fully solvated. Figure 3 shows the scaling behavior of GROMACS for exemplar workloads and its suitability for multi-node executions on Titan: although the simulations of BPTI and NTL9 (14100 atoms when fully solvated) scale sublinearly after 8 cores, 32 cores offer the best relative performance, as measured by execution time.

MD simulations with multiple GROMACS tasks executed on HPC machines can experience large performance fluctuations over the mean runtime values. Such fluctuations would make the separation of RP overheads from resource fluctuations and runtime variations of the application’s tasks difficult, if not impossible. Thus, we profiled and emulated GROMACS simulations with Synapse [28]. Synapse profiles the compute, memory and I/O use of an executable and emulates them. It reproduces the computing activities of an executable, faithfully approximating its time to completion and resource utilization.

Synapse offers our experiments several advantages over the direct use of the executable it emulates: (1) simplified and self-contained deployment without third parties libraries and compilers dependences; (2) high-fidelity replication of the computing patterns of the emulated executable without actual input/output files; (3) profiling capabilities independent of third parties applications; (4) control over the number of FLOPs executed; and (5) selective emulation of the type of profiled resources. As such, Synapse allows greater control, while simplifying deployment and data analysis without loss of generality of results.

We emulated the execution of a single GROMACS instance, simulating BPTI for \( \approx 250 \text{ps} \), the baseline in several studies. In this way, we controlled the runtime noise inherent to executing multiple instances of the same executable: we measured only the variance of Titan and the predictable variance of Synapse. Further, we did not emulate I/O activities as the performance fluctuations of Titan’s network file systems would have dominated our experimental results. Figure 4 shows the narrow distribution of Synapse emulations’ runtime: the mean is 828s with a standard deviation of \( \pm 14 \)s.

Table 1 shows the 8 runs of Experiment 1, designed to measure weak scaling of RP with the chosen workload on Titan. Each run executes between 32 and 4,096 32-cores tasks on a single pilot with between 1,024 and 131,072 cores. The
ratio between the number of tasks executed and the amount of resources acquired is constant across the 8 runs of the experiment. All the tasks are thus executed concurrently in a single so-called ‘generation’, i.e., a single set of concurrent executions. As all the tasks have analogous overheads and all the tasks execute concurrently, the median of the ideal total execution time (TTX) of all the tasks should be analogous for all the 8 runs.

Table 1 shows the 3 runs for Experiment 2, designed to measure the strong scaling of RP with the chosen workload on Titan. Different from Experiment 1, the ratio between number of tasks and number of cores of the pilot varies: Each run executes 16,384 tasks on a single pilot with between 16,384 and 65,536 cores. The rest of the parameters are the same as Experiment 1, each task with a mean execution time of 828s±14 and requiring 32 cores. Because of the disparity between the number of cores required by the tasks and the number of cores of the pilot, the workload is executed on multiple generations, between 32 and 8.

### 4.2 Weak and Strong Scaling

Figure 5 (left) shows the weak scaling of RP for the workload described in Table 1. An ideal TTX (broken line) represents execution time without RP and resource overheads and corresponds to the mean value in Figure 4. In Experiment 1 (Table 1), the ratio between number of tasks and core is constant, enabling fully concurrent executions.

![Graph showing weak scaling](image)

Fig. 5: **Experiments 1 and 2**: Weak (left) and Strong (right) scaling of RADICAL-Pilot.

Figure 5 (left) shows that the actual TTX plotted on the right axes, scales almost linearly between 1,024 and 4,096 cores, and sublinearly between 4,096 and 131,072 cores. The average value of TTX for runs with between 1,024 and 4,096 cores is 922s±14, indicating an average overhead of 11% over the mean of the ideal TTX. This overhead grows to 18% at 8,192, and 160% at 131,072 cores.

| Table 1: Experiments 1 and 2: Weak and strong scalability. |
| --- | --- | --- | --- | --- |
| ID | #Tasks | #Generations | Task Runtime | #Cores/Task | #Cores/Pilot |
| 1 | $2^n, n = [5 - 12]$ | 1 | 828s±14s | 32 | $2^n, n = [10 - 17]$ |
| 2 | $2^{14}$ | $2^n, n = [5 - 3]$ | | | $2^n, n = [14 - 16]$ |
Figure 5 (right) shows that the strong scaling of 16,384 tasks executed from 16,384 to 65,536 cores; this results in the number of generations varying from 32 to 8. When executed over 16,384, 32,816 and 65,536 cores, they have a TTX of 27,794 ± 70, 14,358 ± 259, and 7,612 ± 29 respectively. The deviation from ideal TTX is relatively uniform across different pilot sizes—1,158 ± 150, which indicates that RP is relatively less efficient at higher pilot core counts.

Figures 6 shows the resource utilization (RU) in terms of the percentage of the available core-time spent executing the workload (red), RP code (green), or idling (blue) for Experiment 1 (first 8 bars) and Experiment 2 (last 3 bars). Note the relation between TTX and RU: The more core-time is spent executing the workload, the shorter TTX. Figure 6 shows a relatively constant percentage of core-time utilization for runs with between 32/1024 and 128/4096 tasks/cores, consistent with TTX of Figure 5 (left). The percentage of utilization decreases with the growing of the number of tasks/cores, also consistent with Figure 5 (left).

The last three bars of Figure 6 show progressively shorter values for both RP overhead and idling for runs with multiple generations (as defined in §4.1). When tasks of one generation terminate, those of the following generation immediately starts executing. This eliminates the idling of cores for all generations but the last one. Further, RP overhead increases with the number of cores, indicating that the reduced performance of RP measured in Figure 5 (left) depends, at least to some extent, on the size of the pilot used.

### 4.3 Understanding Weak Scaling

As seen in §3, the RP Agent is implemented with multiple components that can execute concurrently, depending on the workload and the resources on which the Agent is running. Further, multiple instances of the same component can be created to concurrently manage subsets of available tasks and resources. Although distribution and concurrency improve performance, they also make it difficult to determine the underlying causes of sublinear weak scaling.

**Component Concurrency** Figure 7 shows the concurrency of the two main components of the Agent (Scheduler and Executor) and their queues. Concurrency is expressed as the number of tasks managed by each component (or their queue) at any point in time. Each task is initially handled by the Scheduler (Scheduling, Blue); as soon as the required amount of resources for the task become available, it is queued to the Executor (Queuing Executor, Green). Once in the Executor, the task is executed (Executing, Red). Once the execution completes, the task is marked as Done, Cancel or Failed and the Scheduler is informed that resources have been freed (Unscheduling, Purple).
Fig. 7: Task concurrency weak scaling: Scheduler and Executor components.

The Scheduling and Unscheduling operations have concurrency value of 1 because the Scheduler handles one task at a time, and does not retain any tasks in the single-generation setup used for the weak scaling experiment. The time taken to schedule and unschedule tasks (lengths of the blue and purple lines) increases with scale. The number of tasks concurrently queued in the Executor decreases with scale (height of the green line), while the time spent in the queue by the tasks increases (X-value of end of the green line). Similarly, the duration of the plateau (i.e., the maximum number of tasks handled by the Executor as represented by the red line) gets progressively smaller with scale. Figure 7(d) shows that at 4096/131072 cores/tasks, RP does not reach maximum concurrency: the height of red line does not reach 4096 concurrent tasks.

Scheduler and Executor Overheads Figure 8 helps clarify the relation between the performance of the Scheduler and Executor, the two Agent components that appear to contribute to RP overhead. We measure the time spent by each task in each component of the RP Agent. Tasks are pulled from RP DB into Scheduler’s queue (DB Bridge Pulls); after scheduling, the Scheduler queues each task into Executor (Scheduler Queues CU); Executor starts processing the queued task (Executor Starts); the task’s executable starts (Executable Starts) and stops (Executable Stops) executing; and, finally, Executor marks the task as done (CU Spawn Returns).

Fig. 8: Task events weak scaling: Scheduler and Executor components.

Figures 8(a)-(d) shows that all the tasks of the workload, pulled in bulk from the DB (DB Bridge Pulls), enter Scheduler’s queue approximately at the same time (i.e., all the tasks are approximately at the same height compared to the y-axes, forming an almost horizontal line, parallel to the x-axis). The Scheduler takes comparatively more time to schedule the tasks in Figures 8(d) than in Figures 8(a)-(c). Note how the slope of the line formed by the events becomes increasingly steeper from Figures 8(a) to Figures 8(d). The mean scheduling time
for 512 tasks on 16,384 cores is 18s; 39s with 1,024/32,768 tasks/cores; 129s with 2,048/65,536 tasks/cores; and 350s with 4,096/131,072 tasks/cores.

Figures 8(a)-(d) also show two overheads in the Executor: (1) the time spent to prepare a task for its execution (Executor Starts), i.e., the time between when a task is passed to ORTE and when it starts to execute; and (2) the time required for the Executor to be informed that a task has been executed (CU Spawns Return), i.e., the time from when a task stops executing and the time when ORTE passes a message to the Executor about the task Done or Failed state. The mean time to prepare the execution of 512 tasks on 16,384 cores is 37s±9; 37s±6 with 1,024/32,768 tasks/cores; 35s±8 with 2048/65536 cores; and 41s±30 with 4,096/131,072 tasks/cores, which in spite of the high jitter, makes the mean essentially invariant across scales.

The Executor takes variable amount of time to acknowledge that the execution of a task has completed (as given by the timestamp of the CU Spawn Returns event). This variance increases with scale, depending mostly on the time taken by ORTE (i.e., the lunch method used on Titan to execute tasks) to communicate with RP about the task’s state. The distribution of the CU Spawn Returns event is both broad and long-tailed across all the scales. The mean time to communicate the completion of 512 tasks on 16,384 cores is 29s±16; 34s±28 with 1,024/32,768 tasks/cores; 59s±46 with 2048/65536 cores; and 135s±107 with 4,096/131,072 tasks/cores.

**Improving Scheduler Performance** Figure 9 confirms that Scheduler and Executor performance mostly depend on the number of cores of the pilot. Figure 9(a)-(b) show the strong scaling behavior of RP with 32 and 8 generations (corresponding to 32 and 8 “steps” in (a) and (b) respectively), as described in Table 1, Experiment 2. Figure 9(c)-(d) plots the events of one of the 32 generations and those of one of the 8 generations respectively. The Scheduler performance of the strong scaling runs measured: 23s±5 to schedule 512 tasks on 16,384 cores, 28s±13 2048 tasks on 32,768 cores, and 92s±49 2,048 tasks on 65,584 cores. This performance degradation depends on the number of cores, as the number of tasks is constant across Experiment 2 runs. The rate of degradation is similar to what we observed in the weak scaling runs of comparable pilot size.

![Fig. 9: Task events strong scaling: Scheduler and Executor components. Note: Scheduler Queues CU (blue) overlays Executor Starts (orange) events.](image)

Scheduling overhead increases with the number of tasks scheduled: later tasks have to wait longer to be handled, as the Scheduler works sequentially. As a con-
sequence, the performance of the default scheduler of RP decreases with pilot size. This scheduler uses a scheduling approach where a Python data structure representing the resource configuration is repeatedly searched for free cores. This approach is needed and effective for a general purpose scheduler to handle many different kinds of workloads: For example, homogeneous/heterogeneous; MPI/OpenMP/Scalar; and single-node/multi-node. However, as seen in §4.3, the overhead of this approach begin to dominate with more than 128 32-cores tasks and 4096 cores.

To address this, but also to demonstrate the flexibility and extensibility of RP, we implemented a scheduler algorithm which handles the specific workload used in our scaling experiments (homogeneous, multi-node MPI tasks). The implementation of the special purpose scheduler takes as little as 30 lines of code. Its behavior is shown in Figure 10. The scheduler now treats each task in constant time, at a much lower time per task compared to the original scheduler.

We reiterate that this performance improvement comes at the expense of generality, i.e., the scheduler is constrained to handle only homogeneous bag-of-tasks on homogeneous clusters. The loss of generality arises from a change in critical code path from a search to a lookup, which improves the scheduler throughput from 7 tasks/s to 70 tasks/s, an approximately 9 fold improvement over the general purpose scheduler.

5 Discussion and Conclusion

*Prima facie*, a software system implementing the Pilot abstraction [4] provides the conceptual and functional capabilities needed to serve as the runtime system for the scalable execution of a workload comprised of many tasks. The impact of an abstraction is limited to its best implementation. Whereas there are multiple Pilot systems, they are geared towards either specific workloads or platforms. Against this backdrop, RADICAL-Pilot (RP) brings together recent conceptual advances [4] with systems & software engineering [5].

This paper describes RP’s design and implementation (Sec. 3), and characterizes the performance of its Agent module on Titan at the Oak Ridge Leadership Computing Facility (Sec. 4) for workloads comprised of large number of modestly sized MPI tasks. Although RP works on multiple platforms, we focus our experiments on Titan as it currently offers the highest degree of concurrency (300K CPU cores) to researchers in the USA. The experiments discussed in Sec. 4 benefited from RP’s support for introspection and profiling. Using the RADICAL-Analytics toolchain to analyze those profiles, we were able to pinpoint the main contributions to RP’s runtime overhead at scale (more than 40% of Titan).
We demonstrated the extensibility of RP by implementing a simple dedicated scheduler to address a very specific performance bottleneck: the default internal RP scheduler was initially designed for generality, which came at a price in performance. When constraints of generality were removed and the internal scheduler was optimized for homogeneous set of MPI tasks, the performance of the scheduler was significantly enhanced.

When using the optimized scheduler, both the performance and scalability of RP are determined by system software limits. Specifically, we show that the launch rate of tasks is dominated by an overhead arising from the use of OpenMPI Runtime Environment (ORTE) of OpenMPI. Further, we observe that failure rates in the ORTE layer increase significantly when utilizing 131K cores and above. RP stresses ORTE capabilities, however the exact reasons for high jitter in launch rates, and failures after 131K core are currently unknown. Although, current capabilities support production requirements, we continue to work with the ORTE developers to address the observed scalability and stability issues.

The focus of this paper has been on the direct execution of workloads on HPC machines, but RP also forms the middleware and runtime system for a range of other tools and libraries [6–8, 29], already used in production. RP is available for immediate use on many contemporary platforms [30], accompanied with extensive documentation and an active developer-user community.

For molecular sciences, there is an existing and demonstrated need [31] to support up to $10^5$–$10^6$ MPI tasks as part of a single workload. The scalable execution of workloads comprised of many heterogeneous tasks [32] is an increasingly critical requirement (see Ref. [33] for a recent analysis on NERSC systems). These workloads will range from a heterogeneous mix of tasks (both spatial and temporal) to dynamically evolving workloads. RP’s modular architecture and extensible implementation enable us to balance generality and performance, while promoting integration with application tools and system software. As such, we consider RP and its software ecosystem to be well-equipped to support these and future workloads on a wide variety of platforms, including Summit at OLCF.

Software and Data

Source code, raw data and analysis scripts to reproduce experiments can be found at:
RADICAL-Pilot: https://github.com/radical-cybertools/radical.pilot
RADICAL-Analytics: https://github.com/radical-cybertools/radical.analytics
Experiment data and scripts: https://github.com/radical-experiments/rp.paper

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