Probabilistic Diagnosis of Performance Faults in Large-Scale Parallel Applications

ABSTRACT

Debugging large-scale parallel applications is challenging. Most existing techniques provide mechanisms for process control, but they provide little information about the causes of failures. Most debuggers also scale poorly despite continued growth in supercomputer core counts. We have developed a novel, highly scalable tool to help developers understand and fix correctness problems at scale. Our tool probabilistically infers the least progressed task in MPI programs using Markov models of execution history and dependence analysis. This analysis guides program slicing to find code that may have caused a failure. In a blind study, we demonstrate that our tool can isolate the root cause of a particularly perplexing bug encountered at scale in a molecular dynamics simulation. Further, we perform fault injections into two benchmark codes and measure the scalability of the tool. Our results show that it accurately detects the least progressed task in most cases and can perform the diagnosis in a fraction of a second with thousands of tasks.

1. INTRODUCTION

Debugging errors and abnormal conditions in large-scale parallel applications is difficult. While High Performance Computing (HPC) applications have grown in complexity and scale, debugging tools have not kept up. Most tools cannot scale to the process counts of the largest systems. More importantly, most tools provide little insight into the causes of failures. The situation is particularly challenging for performance faults (e.g. slow code regions and hangs), which may manifest in different code or on a different process from their causes.

We present *PDI* (*Progress-Dependence Inference*), a tool that provides insight into performance faults in large-scale parallel applications[1]. *PDI* probabilistically identifies the *least progressed (LP) task* (or tasks) in parallel code. *PDI* uses a Markov Model (MM) as a lightweight, statistical summary of each task's control-flow history. MM states represent MPI calls and computation, and edges represent transfer of control. This model lets us tie faults to locations in the code. However, in parallel applications, faults may lie on separate tasks from their root causes, so we introduce *progress dependence* to diagnose performance faults in parallel applications. We create a *progress dependence graph* (PDG) to capture wait chains of non-faulty tasks whose progress depends on the faulty task. We use these chains to find the LP task in parallel. Once we find the LP task, *PDI* then applies program slicing [33] on the task's state to identify code that may have caused it to fail.

To ensure scalability, we use a novel, fully distributed algorithm to create the PDG. Our algorithm uses minimal per-task information, and it incurs only slight runtime overhead for the applications we tested. Our implementation of *PDI* is non-intrusive, using the MPI profiling interface to intercept communication calls, and it does not require separate daemons to trace the application as do other tools (e.g., TotalView [25], STAT [5]).

This paper makes the following contributions:

- The concept of progress dependence between tasks and its use for diagnosing performance faults;
- A scalable, distributed, probabilistic algorithm for creating a progress dependence graph and discovering the least progressed task;
- A practical way to apply backward slicing to find the origin of a fault from the state of the least progressed task in a faulty execution.

We evaluate *PDI* by performing fault injection on AMG2006 and LAMMPS, two of the ASC Sequoia benchmarks. *PDI* finds a faulty task in a fraction of a second on up to 32,768 tasks. *PDI* accurately identifies the LP task 88% of the time, with perfect precision 86% of the time. We show that *PDI* can diagnose a difficult bug in a molecular dynamics code [27] that manifested only with 7,996 or more processes. *PDI* quickly found the fault — a sophisticated deadlock condition.

The rest of the paper is organized as follows. Section 2 presents an overview of our approach and Sections 3 and 4 detail our design and implementation. Section 5 presents our case study and fault injection experiments. In Section 7 we state our conclusions.

[1] A failure is a deviation from specification, while a fault may cause failures. A hang is a failure, while a fault is a code segment that sends an incorrect message.

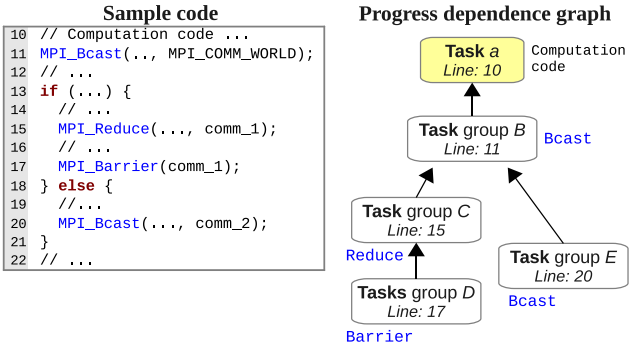


Figure 1: Progress dependence graph example.

2. OVERVIEW OF THE APPROACH

2.1 Progress Dependence Graph

A *progress-dependence graph* (PDG) represents dependencies that prevent tasks from making further execution progress at any given point in time. A PDG facilitates pinpointing performance faults that cause failures such as program stalls, deadlocks and slow code regions, and in performance tuning the application (e.g., by highlighting tasks with the least progress).

A PDG starts with the observation that two or more tasks must execute an MPI collective in order for (all of) them to move forward in the execution flow. For example, `MPI_Reduce` is often implemented in MPI using a binomial tree for short messages [29]. Since the MPI standard does not require collectives to be synchronizing, some task could enter and leave this state — the `MPI_Reduce` function call — while others remain in it. Tasks that only send messages in the binomial tree enter and leave this state, while tasks that receive (and later send) messages block in this state until the corresponding sender arrives. These blocked tasks are *progress dependent* on other (possibly delayed) tasks.

This definition formalizes progress dependence: *Let the set of tasks that participate in a collective operation be X. If a task subset $Y \subseteq X$ has reached the collective operation while another tasks subset $Z \subseteq X$, where $X = Y \cup Z$ has not yet reached it at time t such that the tasks in Y blocked at t waiting for tasks in Z then Y is progress-dependent on Z, which we denote as $Y \xrightarrow{pd} Z$.*

Figure 1 shows an example PDG in which task a blocks in (computation code) line 10. Task a could block for many reasons, such as a deadlock due to incorrect thread-level synchronization. As a consequence, a group of tasks B block in `MPI_Bcast` in line 11 while other tasks proceed to other code regions — tasks group C, D and E block in code lines 15, 17, and 20. No progress-dependence exists between groups C and E because they are in different execution branches.

Point-to-Point Operations: In blocking point-to-point operations such as `MPI_Send` and `MPI_Recv`, the dependence is only on the peer task which we formalize as follows: *If task x blocks when sending (receiving) a message to (from) task y at time t then x is progress dependent on y, i.e., $x \xrightarrow{pd} y$.* This definition also applies to nonblocking operations such as `MPI_Isend` and `MPI_Irecv`. The main difference is that the dependence does not apply directly to the send (or receive) operation, but to the associated completion (e.g., a wait or test operation). If a task x blocks on `MPI_Wait`, for example, we infer the task y, on which x is progress dependent, from the request on which x waits. Similarly, if x spins on a test, for example by calling `MPI_Test`, we infer the peer task on which x is progress dependent from the associated request. On the receiving end, we can also infer the dependence from other test operations such as `MPI_Probe` or `MPI_Iprobe`. In any case, we denote the progress dependence as $x \xrightarrow{pd} y$.

PDG-Based Diagnosis: A PDG can intuitively pinpoint the task (or task group) that originates a performance failure. In Figure 1, task a can be blamed for originating the program's stall since it has no progress dependence on any other task (or group of tasks) in the PDG. It is also the least progressed (LP) task.

From the programmer's perspective, the PDG provides useful information in debugging, testing and performance tuning. First, given a performance failure such as the one in Figure 1, the PDG directly shows where to focus attention, i.e., the LP tasks. Thus, debugging time is substantially reduced, as the programmer can now focus on the execution context of one (or a few) task(s) rather than on possibly thousands of tasks. Second, we can efficiently apply static or dynamic bug-detection techniques based on the state of the LP tasks. *PDI* applies program slicing [33] using the state of the LP task (e.g., stack variables and program counter) as initial criterion, which substantially reduces the search space of program slicing when compared to slicing the execution context of each task (or representative task group) separately and then combining this information to try to find the fault.

PDG Versus Other Dependency Graphs: A PDG is different from the dependency graph used in MPI deadlock detection [17, 18, 30]. A PDG hierarchically describes the execution progress of MPI tasks. It addresses questions such as: What is the task with the least progress? Which tasks does the LP task prevent from making progress? In contrast, traditional dependency graphs can detect real and potential deadlocks by searching for knots in the graph. We do not detect deadlocks by checking for knots in a PDG. However, since a PDG combines dependencies arising from MPI operations, it can indicate that a deadlock caused a hang. Performance failures are a superset of hangs; deadlocks or other causes can lead to hangs. Our case study with a real-world bug in Section 5.1 shows an example in

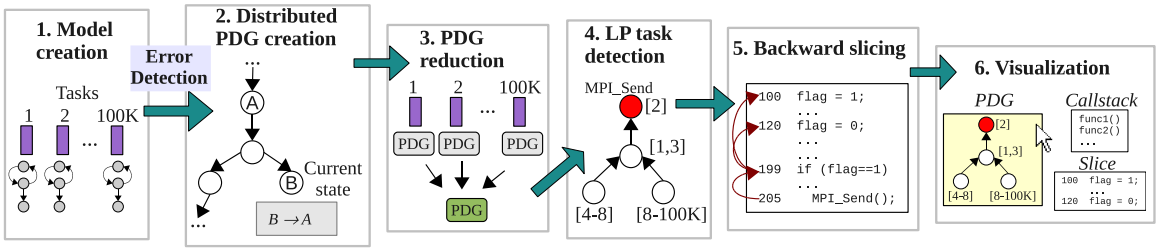


Figure 2: Overview of the diagnosis work flow.

which we use a PDG to identify that a deadlock was the root-cause of a hang.

2.2 Workflow of Our Approach

Figure 2 shows the steps in *PDI* to diagnose performance problems. Steps 1–3 are distributed while steps 4–6 are performed in a single task.

(1) Model creation. *PDI* captures per-MPI-task control-flow behavior in a Markov model (MM). MM states correspond to two code region types: *communication* regions, i.e., code executed within an MPI function; and *computation* regions, i.e., code executed between two MPI functions. Other work uses similar Markov-like models (in particular semi-Markov models) to find similarities between tasks to detect errors [9, 22]. *PDI* instead uses MMs to summarize control-flow execution history. To the best of our knowledge, no prior work uses MMs to infer progress dependencies.

(2) Distributed PDG creation. When a system detects a performance fault (either *PDI* or a third-party system), *PDI* uses a distributed algorithm to create a PDG in each task. First, we use an all-reduce over the MM state of each task, which provides each task with the state of all other tasks. Formally, if a task's local state is s_{local}, this operation provides each task with the set $S_{\text{others}} = s_1, \ldots, s_j, \ldots, s_N$, where $s_j \neq s_{\text{local}}$. Next, each task probabilistically infers its own local PDG based on s_{local} and S_{others}.

(3) PDG reduction. Our next step reduces the PDGs from step (2) to a single PDG in a distributed manner. The reduction operation is the union of edges in two PDGs, i.e., the union (in each step of the reduction) of progress dependencies.

(4) LP task detection. Based on the reduced PDG, we determine the LP task and its state (i.e., call stack and program counter), which we use in the next step.

(5) Backward slicing. We then perform backward slicing using Dyninst [3]. This step finds code that could have led the LP task to reach its current state.

(6) Visualization. Finally, *PDI* presents the program slice, the reduced PDG and its associated information. The user can attach a serial of parallel debugger to the LP task based on the PDG. The slice brings programmers' attention to code that affected the LP task, and allows them to find the fault.

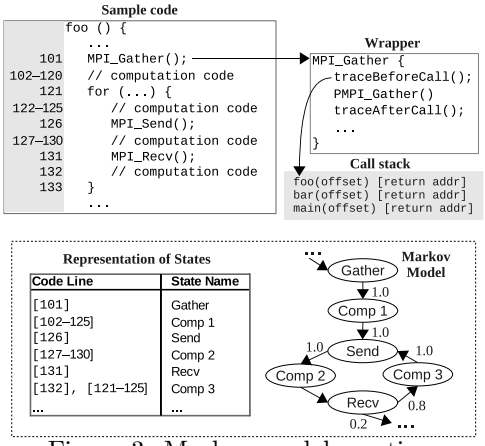


Figure 3: Markov model creation.

3. DESIGN

3.1 Summarizing Execution History

A simple approach to save the control-flow execution history directly might build a control-flow graph (CFG) based on executed statements [19]. Since large-scale MPI applications can have very large CFGs, *PDI* instead captures a compressed version of the control-flow behavior using our MM with communication and computation states. The edge weights capture the frequency of transitions between two states. Figure 3 shows how *PDI* creates MMs at runtime in each task. We use the MPI profiling interface to intercept MPI routines. Before and after calling the corresponding PMPI routine, *PDI* captures information such as the call stack, offset address within each active function and return address. We assume that the MPI program is compiled using debugging information so that we can resolve function names.

3.2 Progress Dependence Inference

In this section, we discuss how we infer progress dependence from our MMs. For simplicity, we restrict the discussion to dependencies that arise from collective operations. The process is similar for point-to-point operations although the MM states in the following discussion must reflect send/receive relationships. *PDI* probabilistically infers progress dependence between a task's

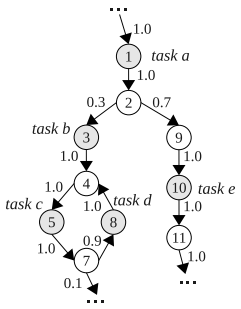


Figure 4: Sample MM with five blocked tasks.

Table 1: Dependence based on path probabilities.

$P(i,j)$			$P(j,i)$				
0	$0 < P < 1$	1	0	$0 < P < 1$	1	Dependence?	Type
✓			✓			No	
✓				✓		Yes	$t_i \xrightarrow{pd} t_j$
✓					✓	Yes	$t_i \xrightarrow{pd} t_j$
	✓		✓			Yes	$t_i \xleftarrow{pd} t_j$
	✓			✓		?	
	✓				✓	Yes	$t_i \xrightarrow{pd} t_j$
		✓	✓			Yes	$t_i \xleftarrow{pd} t_j$
		✓		✓		Yes	$t_i \xleftarrow{pd} t_j$
		✓			✓	?	

local state and the states of other tasks. Intuitively, our MM models the probability of going from state x to state y via *some* path $x \rightsquigarrow y$. If a task t_x in x must eventually reach y with high probability then we can determine that a task t_y in state y could be waiting for t_x in which case we infer that $y \xrightarrow{pd} x$.[2]

Figure 4 illustrates how we infer progress dependence from our MMs. Five tasks (a, b, c, d and e) are blocked in different states (1, 3, 5, 8, and 10 respectively). To estimate the progress dependence between task b and task c, we calculate that the path probability $P(3, 5)$, the probability of going from state 3 to state 5 over all possible paths, which is 1.0. Thus, *task c is likely to be waiting for task b, since according to the observed execution, if a task is in state 3 it always must reach state 5.* To estimate progress dependence more accurately, we consider the possibility of loops and evaluate the backward path probability $P(5, 3)$, which in this case is zero. Thus, task c cannot reach task b, so we can consider it to have progressed further than task b so $c \xrightarrow{pd} b$.

Resolving conflicting probability values. When a backward path probability $P(j, i)$ is zero, a task in state j has made more progress than a task in state i. However, if the forward path probability $P(i, j)$ is 1.0 and the backward path probability is nonzero then the task in state j might return to i. For example, for tasks d and c in Figure 4, $P(8, 5) = 1.0$ but $P(5, 8) = 0.9$. In this case, task d must eventually reach state 5 to exit the loop so we estimate that $c \xrightarrow{pd} d$; our results demonstrate that this heuristic works well in practice.

The dependence between task b and task e is null, i.e., no progress dependence exists between them. They are in different execution branches so the forward and backward path probabilities between their states, i.e., $P(3, 10)$ and $P(10, 3)$, are both zero. The same holds for the dependencies between task e and task c or d.

General progress dependence estimation. To estimate the progress dependence between tasks t_i and t_j in states i and j, we calculate two path probabilities: (i) a forward path probability $P(i, j)$; and (ii) a backward path probability $P(j, i)$. A path probability is the likelihood of going from one state to another over all possible paths. We use Table 1 to estimate progress dependencies. If both probabilities are zero (i.e., the tasks are in different execution branches), no dependence exists between the tasks. When one probability is 1.0 and the other is less than 1.0, the first *predominates* the second. Therefore, the second probability determines the dependence. For example, if the second is $P(j, i)$ we determine $t_j \xrightarrow{pd} t_i$ since execution goes from i to j. If one probability is zero and the second is nonzero, then the second predominates the first. Therefore, the first probability determines the dependence. For example, if the first is $P(i, j)$ we determine $t_i \xrightarrow{pd} t_j$ because execution could go from j to i but not from i to j.

We cannot determine progress dependence for two cases: when both probabilities are 1.0; and when both probabilities are in the range $0.0 < P < 1.0$. The first case could happen when two tasks are inside a loop and, due to an error, they do not leave the loop and block inside it. In this case both backward and forward path probabilities are 1.0, so it is an undefined situation. The probabilities in the second case simply do not provide enough information to decide. For these cases, *PDI* marks the edges in the PDG as undefined so that the user knows that the relationship could not be determined. These cases occur infrequently in our experimental evaluation. When they do, the user can usually determine the LP task by looking at tasks that are in one group or cluster. Section 5 gives examples of how the user can resolve these cases visually.

Algorithm. Figure 5 shows our local PDG construction algorithm, which takes an MM and *statesSet*, the states of all other tasks as input. We compute the dependency between the local state and *statesSet*. We represent dependencies as integers (0: no dependence; 1: forward dependence; 2: backward dependence; 3: undefined). We save the PDG in an adjacency matrix. The function `dependence` determines dependencies based on all-path probabilities (calculated in `probability`) and Table 1 (captured in `dependenceBasedOnTable`).

The overall complexity of the algorithm is $O(s \times (|V| +$

[2]For simplicity, we also represent progress dependencies in terms of the states in which the tasks are.

```
1  Input: mm (Markov model),closure (transitive closure
2 of the mm), statesSet (set of states)
3 Output: depMatrix (PDG adjacency-matrix representation)
4
5 progressDependenceGraph() { /* Builds PDG */
6   State localState ← getLocalState(mm)
7   for each State s in statesSet
8     if s is not localState {
9       d ← dependence(localState, s)
10      depMatrix[localState, s] ← d
11    }
12 }
13
14 /* Calculates dependence between two states */
15 dependence(State src, State dst) {
16   p ← probability(src, dst)
17   d ← dependenceBasedOnTable(p)
18   return d
19 }
20
21 /* Calculates reachability probability */
22 probability(State src, State dst) {
23   p ← 0
24   if src can reach dst in closure {
25     for each Path p between src and dst
26       p ← p + pathProbability(src, dst)
27   }
28   return p
29 }
```

Figure 5: Algorithm to create the PDG.

$|E|$)), where s is the number of states in *statesSet*, and $|V|$ and $|E|$ are the numbers of states and edges of the MM. In practice, the MMs are sparse graphs in which $|E| \approx |V|$, so the complexity is approximately $O(s \times |E|)$.

Comparison to postdominance. Our definition of progress dependence is similar to the concept of postdominance [12] in which a node j of a CFG postdominates a node i if every path from i to the *exit* node includes j. However, our definition does not require the *exit* node to be in the MM (postdominance algorithms require it to create a postdominator tree). Since a fault could cause the program to stop in any state, we are not guaranteed to have an exit node within a loop. Techniques such as assigning a dummy exit node to a loop do not work in general for fault diagnosis because a faulty execution makes it difficult (or impossible) to determine the right exit node. In order to use postdominance theory, we could use static analysis to find the exit node and map it to a state in the MM. However, our dynamic analysis approach is more robust and should provide greater scalability and performance.

4. SCALABLE PDG-BASED ANALYSIS

PDI is implemented in C++ and uses the Boost Graph Library [2] for graph-related algorithms such as depth-first search. In this section, we focus on the implementation details that ensure scalability.

4.1 Error Detection

We assume that a performance problem has been detected, for example, because the application is not producing the expected output in a timely manner. The user can then use *PDI* to find the tasks and the associated code region that caused the problem. *PDI* includes a timeout detection mechanism that can trigger the diagnosis analysis, and it can infer a reasonable timeout threshold (based on the mean time and standard deviation of state transitions). The user can also supply the timeout as an input parameter. Our experiments with large-scale HPC applications found that a 60 second threshold is sufficient.

Table 2: Some examples of dependence unions.

No	Task x	Task y	Union	Reasoning	OR operation
1	$i \to j$	null	$i \to j$	first dependence dominates	$1 + 0 = 1$
2	$i \to j$	$i \to j$	$i \to j$	same dependence	$1 + 1 = 1$
3	$i \leftarrow j$	$i \leftarrow j$	$i \leftarrow j$	same dependence	$2 + 2 = 2$
4	$i \to j$	$i \leftarrow j$	$i?j$	undefined	$1 + 2 = 3$
5	null	null	null	no dependence	$0 + 0 = 0$

4.2 Distributed Inference of the PDG

Helper thread. *PDI* uses a helper thread to perform its analysis of the MM, which is built in the main thread. Steps 2–3, which are shown in Figure 2 and are the core of the dependence inference, are distributed while Steps 4–6, are inexpensive operations that only one task performs (MPI rank 0 by default). *PDI* uses `MPI_THREAD_MULTIPLE` to initialize MPI so that multiple threads can call MPI. On machines that do not support threads, such as BlueGene/L, we save the MM to the parallel file system when we detect an error. *PDI* then reads the MM of each process in a separate MPI program to perform the analysis.

Distributed algorithm. The following steps provide more detail of steps 2–3 in the workflow:
(1) We first perform a reduction over the current state of all tasks to compute the *statesSet* of all tasks.
(2) We next broadcast *statesSet* to all tasks.
(3) Each task uses the algorithm in Figure 5 to compute its local PDG from its local state and *statesSet*.
(4) Finally, we perform a reduction of the local PDGs to calculate the union of the edges (forward or backward). Table 2 shows examples of some union results. In case 1, a dependence is present in only one task so the dependence predominates. In cases 2 and 3, the dependencies are similar so we retain it. In case 4, they conflict so the resulting dependence is undefined. We efficiently implement this operator using bitwise `OR` since we represent dependencies as integers.

We cannot use `MPI_Reduce` for our reduction steps (for example, tasks can contribute states of different sizes) so we implement custom reductions that use binomial trees. These operations have $O(\log p)$ complexity where p is the number of tasks. Assuming a scalable broadcast implementation, the overall complexity is also $O(\log p)$. Our algorithm can therefore scale to the task counts found on even the largest HPC systems.

4.3 Determination of LP Task

We compute the LP task (or task group) from the reduced PDG. *PDI* first finds nodes with no outgoing edges based on dependencies from collectives and marked them as LP. If more than one node are found, *PDI* discards nodes that have point-to-point dependencies on other non-LP tasks in different branches. Since *PDI* operates on a probabilistic framework (rather than on deterministic methods [5]), it can incorrectly pinpoint the LP task, although such errors are rare according to our evaluation. However, in most of these cases, the user can still determine the LP task by visually examining the PDG (by looking for nodes with only one task).

4.4 Guided Application of Program Slicing

Background. Program slicing transforms a large program into a smaller one that contains only statements that are relevant to a particular variable or statement. For debugging, we only care about statements that could have led to the failure. However, message-passing programs complicate program slicing since we must reflect dependencies related to message operations.

We can compute a program slice statically or dynamically. We can use static data and control flow analysis to compute a static slice [33], which is valid for all possible executions. Dynamic slicing [21] only considers a particular execution so it produces smaller and more accurate slices for debugging.

Most slicing techniques that have been proposed for debugging message-passing programs are based on dynamic slicing [20, 24, 26]. However, dynamically slicing of a message-passing program usually does not scale well. Most proposed techniques have complexity at least $O(p)$. Further, the dynamic approach suffers high costs to generate traces of each task (typically by code instrumentation) and to aggregate those traces centrally to construct the slice. Some approaches reduce the size of dynamic slices by using a global predicate rather than a variable [24, 26]. However, the violation of the global predicate may not provide sufficient information to diagnose failures in complex MPI programs.

We can use static slicing if we allow some inaccuracy. However, we cannot naively apply data-flow analysis (which slicing uses) in message-passing programs [28]. For example, consider the following code fragment:

```
1  program() {
2    ...
3    if (rank == 0) {
4      x = 10;
5      MPI_Send(...,&x,...);
6    } else {
7      MPI_Recv(...,&y,...);
8      result = y * z;
9      printf(result);
10     ...
```

Traditional slicing on `result` in line 9 identifies statements 7, 8, and 9 as the only statements in the slice, but statements 3–9 should be in the slice. Statements 4-5 should be in the slice because the value x sent is received as y which obviously influences z. Thus, we must consider the SPMD nature of the program in order to capture communication dependencies. The major problem with this *communication-aware slicing* is the high cost of analyzing a large dependence graph [28] to construct a slice based on a particular statement or variable. Further, the MPI developer must decide on which tasks to apply communication-aware static slicing since applying it to every task is infeasible at large scales.

Approach. *PDI* progressively applies slicing to the execution context of tasks that are representative of behavioral groups, starting with the groups that are most relevant to the failure based on the PDG. *PDI* uses the following algorithm:
(1) Initialize an empty slice S.
(2) Iterate over PDG nodes from the node corresponding to the LP task to nodes that depend on it, and so on to the leaf nodes (i.e., the most progressed tasks).
(3) In each iteration i, $S = S \bigcup s_i$ where s_i is the statement set produced from the state of a task in node i.

This slicing method reduces the complexity of manually applying static slicing to diagnose a failure. The user can simply start with the most important slice (i.e., the one associated with the LP task) and progressively augment it by clicking the "next" button in a graphical interface, until the fault is found.

5. EVALUATION

5.1 Case Study

An application scientist challenged us to locate an elusive error in ddcMD, a parallel classical molecular-dynamic code [27]. This was a hang that emerges intermittently only when run on Blue Gene/L with 7,996 MPI tasks. Although he had already identified and fixed the error after significant time and effort, he hoped that we could provide a technique that would not require tens of hours. In this section, we present a blind case study, in which we were supplied no details of the error, that demonstrates *PDI* can efficiently locate faults.

Figure 6 shows the result of our analysis. Our tool first detects the hang condition when the code stops making progress, which triggers the PDG analysis to identify MPI task 3,136 as the LP task — *PDI* first detects tasks 3,136 and 6,840 as LP tasks and then eliminates 6,840 since it is point-to-point dependent on task 0, a non-LP task, in the left branch. The LP task in the `a` state, causes tasks in the `b` state that immediately depend on its progress to block, ultimately leading to a global stall through the chain of progress dependencies. This analysis step reveals that task 3,136 stops progressing as it waits on an `MPI_Recv` within the `Pclose_forWrite` function. Once it identifies the LP

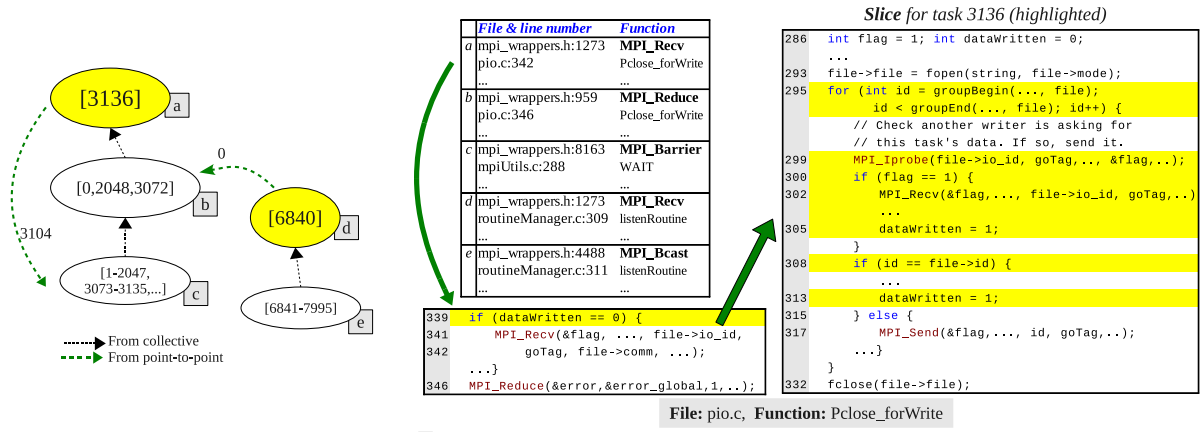


Figure 6: Output for ddcMD bug.

task, *PDI* applies backward slicing starting from the `a` state, which identifies `dataWritten` as the data variable that most immediate pertains to the current point of execution. Slicing then highlights all statements that could directly or indirectly have affected its state.

The application scientist verified that our analysis precisely identified the location of the fault. ddcMD implements a user-level, buffered file I/O layer called `pio`. MPI tasks call various `pio` functions to move their output to local per-task buffers and later call `Pclose_forWrite` to flush them out to the parallel file system. Further, in order to avoid an I/O storm at large scales, `pio` organizes tasks into I/O groups. Within each group, one writer task performs the actual file I/O on behalf of all other group members. A race condition in the complex writer nomination algorithm — optimized for a platform-specific I/O forwarding constraint — and overlapping consecutive I/O operations causes the intermittent hang. The application scientist stated that the LP task identification and highlighted statements would have provided him with critical insight about the error. He further verified that a highlighted statement was the bug site.

More specifically, on Blue Gene/L, a number of compute nodes perform their file I/O through a dedicated I/O node (ION) so `pio` nominates *only one* writer task per ION. Thus, depending on how MPI tasks map to the underlying IONs, an I/O group does not always contain its writer task. In this case, `pio` instead nominates a non-member task that belongs to a different I/O group. This mechanism led to a condition in which a task plays dual roles: a non-writer for its own I/O group and the writer for a different group.

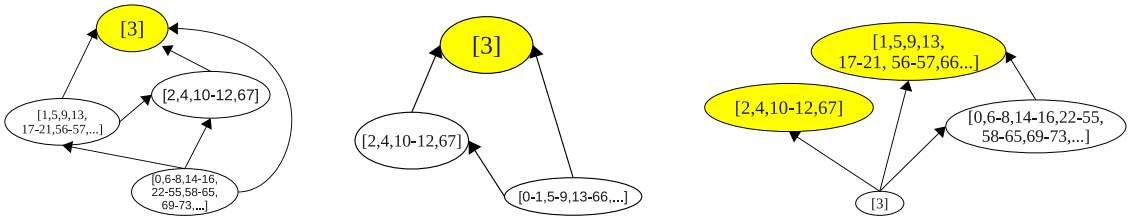
Figure 6 shows the main loop of a writer. To receive the file buffer from a non-writer, the group writer first sends to each of its group members a request to send the file buffer via the `MPI_Send` at line 317. The group member receives that request via the `MPI_Recv` at line 341 and sends back the buffer size and the buffer. As shown in the loop, a dual-purpose task has an extra logic: it uses `MPI_Iprobe` to test whether it must reply to its non-writer duty while it performs its writer duty. The logic is introduced in part to improve performance. However, completing that non-writer duty frees its associated writer task to move on from MPI blocking communications. The hang arises when two independent instances of `pio` are simultaneously processing two separate sets of buffers. This pattern occurs in the application when a small data set is written immediately after a large data set. Some tasks can still be performing communication for a large data set while others work on a small set. Because the MPI send/recv operations use tags that are fixed at compile time, messages from a small set could be confused for those for a large set of `pio` and vice-versa, leading to a condition in which a task could hang waiting for a message that was intercepted by a wrong instance.

This error only arose on this particular platform because the dual-purpose condition only occurs under Blue Gene's unique I/O forwarding structure. We also theorize that the error emerges only at large scales because this scale increases the probability that the dual-purpose assignments and simultaneous `pio` instances occur. The application scientist had corrected the error through unique MPI tags in order to isolate one `pio` instance from another.

5.2 Fault injections

Applications. To evaluate *PDI*, we inject faults into two Sequoia benchmarks: AMG2006 and LAMMPS [1]. These codes are representative of large-scale HPC production workloads. AMG2006 is a scalable iterative solver for large structured sparse linear systems. LAM-MPS is a classical molecular dynamics code. For AMG-2006, we use the default 3D problem (test 1) with the same size in each dimension. For LAMMPS, we use "crack", a crack propagation example in a 2D solid.

Injections. We inject a local application hang by



(a) hypre_ParVectorCopy (b) hypre_CSRMatrixMatvec (c) MPI_Irecv

Figure 7: Examples of PDGs indicating LP tasks (highlighted) for AMG2006. Errors are injected in task 3.

making a randomly selected process suspend execution for a long period to activate the timeout error detection mechanism in *PDI*. We use Dyninst [3] to inject the fault into the application binaries as a sleep call at the beginning of randomly selected function calls (20 user, 5 MPI). Our injector first profiles a run of the application so that we randomly choose from functions that are used during the run. We use a higher proportion of user function calls because more user functions than MPI functions are used at runtime. These function calls capture a wide range of program behaviors including calls inside complex loops as well as ones at the beginning or end of the program. We perform all fault-injection experiments on a Linux cluster with nodes that have six 2.8 GHz Intel Xeon processors and 24 GB of RAM. We use 1,000 tasks in each run.

Coverage results. We use three metrics to evaluate diagnosis quality: *LPT detection recall*, the fraction of cases in which the set of LP tasks that *PDI* finds includes the faulty task; *isolation*, the fraction of cases in which the faulty task is not detected but it is the only task in a PDG node (i.e. a singleton task); and *imprecision*: the percentage of the total number of tasks in the LP task set that *PDI* finds that are not LP tasks; we should have only one task in the set since we inject in a single task. Figure 7(a)-(b) shows two cases of correct LPT detections, which should have only the one task into which we inject the error for these experiments. A singleton task appears suspicious to a user so we consider isolation as semi-successful. Figure 7(c) shows an example of isolation — the PDG isolates faulty task (3).

PDI detects the LP task accurately most of the time (for AMG2006, all 20 user calls and 2 MPI calls; for LAMMPS, 19 user calls and 3 MPI calls). *PDI* isolates the LP task in all cases that it is not detected. *PDI* has very low imprecision: 43 (out of 50) injections resulted in no incorrect tasks in the LP set. Only one AMG2006 case gives high imprecision (0.99) since progress dependencies are undetermined (and the PDG had only one node). Three remaining cases had low imprecision of 0.01 to 0.05. LPT detection recall is higher for user calls than MPI calls because if a task blocks in a computation region, the remaining tasks are likely to block in the next communication region, which follows the computation region in our MM with probability one

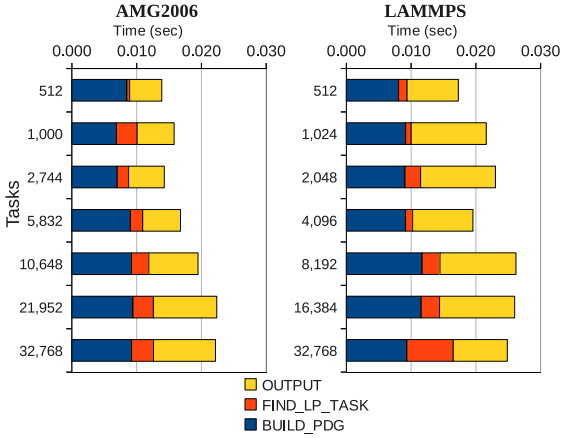


Figure 8: Time to perform distributed analysis (steps 2–4 in workflow) on BlueGene/P.

and, thus, *PDI* is likely to detect the dependence. Alternatively, if a task blocks in a communication region, the other tasks likely block in another communication region, which is necessarily not an adjacent MM state so *PDI* has a lower probability of finding the LP task. Nonetheless, *PDI* isolates the faulty task in all cases that it does not correctly detect the LP task.

5.3 Performance

Scalability We run AMG2006 and LAMMPS up to 32,768 MPI tasks on an IBM BlueGene/P system and measure the time that *PDI* takes to perform the distributed part of its analysis (i.e., steps 2–4 in its workflow). In each code, we inject an error close to its final execution phase in order to have the largest possible MM (to stress *PDI* with the largest input graph). We used BlueGene/P's smp mode in which each node has one MPI task with up to four threads.

Figure 8 shows the results of these experiments. In each run, we measure three main steps: `BUILD_PDG` (steps 2 and 3; `FIND_LP_TASK` (the first part of step 4 in which the helper thread identifies the LP task); `OUTPUT` (the second part of step 4, which post-processes the final PDG). In `OUTPUT`, *PDI* eliminates duplicate edges in the PDG that may result from the distributed merging process of PDGs. It also groups MPI task ranks into ranges of the form [x–y] and adds these ranges to the corresponding PDG nodes. Figure 8 shows that

Table 3: Slowdown and Memory usage.

Benchmark	Slowdown	Memory usage
LAMMPS	1.59	6.11
AMG2006	1.46	10.36
BT	1.08	3.75
SP	1.67	5.14
CG	1.14	2.21
FT	1.05	1.01
LU	1.39	5.37
MG	1.04	1.04

`FIND_LP_TASK` contributes the least to the analysis overhead. Intuitively, finding the LP task is simple once we have built the PDG. `BUILD_PDG` is the core of the analysis and, so, accounts for the most overhead. Our results demonstrate the scalability of *PDI*. The distributed analysis takes less than a second on up to 32,768 MPI tasks. The low cost of this analysis suggests that we can trigger it at multiple execution points with minimal impact on the application run.

Slowdown and memory usage. Table 3 shows application slowdown and *PDI* memory usage for AMG-2006, LAMMPS, and six NAS Parallel benchmarks: BT, SP, CG, FT, LU and MG [7]. We omit EP because it performs almost no MPI communication and IS because it uses MPI only in a few code locations. Since their MPI profiles produce small MMs, monitoring at the granularity of MPI calls does not suit these applications. Slowdown is the ratio of the application run time with *PDI* to the run time without it. Memory usage shows the increase in program heap usage when we use *PDI*. Since tasks can have different memory usage (depending on their behavior), we used the task with the highest memory usage. *PDI* incurs little slowdown – the worst is 1.59 for LAMMPS – because the overhead is primarily the cost of intercepting MPI calls and updating the MM, steps that we have highly optimized. For example, to optimize MM creation, we use efficient C++ data structures and algorithms such as associative containers and use pointer comparisons (rather than string-based comparisons) to compare states. Memory usage is moderate for most benchmarks; the largest is AMG2006 (10.36), which has many (unique) states in its execution.

6. RELATED WORK

The traditional debugging paradigm [6, 15, 25] of interactively tracking execution of code lines and inspecting program state does not scale to existing high-end systems. Recent efforts has focused on improving the scalability of tools that realize this paradigm [6, 10]. Ladebug [8] and the PTP debugger [32] also share the same goal. While these efforts enhanced debuggers to handle increased MPI concurrency, root cause identification is still a time consuming, manual process.

Automated root-cause analysis tools have begun to target general coding errors in large-scale scientific computing. Research work includes probabilistic tools [13, 9, 22, 23] that detect errors through deviations of application behavior from a model. AutomaDeD [22] and Mirgorodskiy et al. [23] both monitor the application's timing behaviors and focus the developer on tasks and code regions that exhibit unusual behaviors. More common tools target specific error types, such as memory leaks [16] or MPI coding errors [13, 14, 17, 18, 30]. These tools are complimentary to *PDI* as they can detect a problem and trigger *PDI*'s diagnosis mechanisms.

Assertion-based debugging also targets reduced manual effort. Recent work addressed scalability challenges of parallel assertion-based debugging [11] but it is not well suited for localizing performance faults. Differential debugging [4] provides a semi-automated approach to understand programming errors; it dynamically compares correct and incorrect runs. While these techniques have been applied at small scales [31], the time and scale expenses are likely prohibitive at large scales.

The closest prior work to *PDI* is STAT [5], which provides scalable detection of task behavioral equivalence classes based on call stack traces. Its temporal ordering relates tasks by their logical execution order so a developer can identify the least- or most-progressed tasks. However, STAT primarily targets assisting developers in the use of traditional debuggers. In contrast, *PDI* monitors the execution of the program to detect abnormal conditions and locate the fault automatically.

Others have explored program slicing in MPI programs to locate code sites that may lead to errors. To provide higher accuracy, most techniques use dynamic slicing [20, 24, 26]. These tools tend to incur large runtime overheads and do not scale. Also, techniques must include communication dependencies into data-flow analysis, which is also expensive, to avoid misleading results. *PDI* uses other information to limit the use of slicing in order to limit overhead.

7. CONCLUSIONS

Our novel debugging approach can diagnose faults in large-scale parallel applications. By compressing historic control-flow behavior of MPI tasks using Markov models, our technique can identify the least progressed task of a parallel program by inferring probabilistically a progress-dependence graph. Using backward slicing, our approach pinpoints code that could have led the offending task to reach its unsafe state. We design and implement *PDI*, which uses this approach to diagnose the most significant root-cause of a problem. Our analysis of a hard-to-diagnose bug and fault injections in three representative large-scale HPC applications demonstrate the utility and significance of *PDI*, which identifies these problems with high accuracy, where manual analysis and traditional debugging tools have been unsuccessful. The distributed part of the analy-

sis is performed in a fraction of a second with over 32 thousand tasks. The low cost of the analysis allows its use at multiple points during program execution.

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