Techniques for Efficiently Querying Scientific Workflow Provenance Graphs

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ABSTRACT

A key advantage of scientific workflow systems over traditional scripting approaches is their ability to automatically record data and process dependencies introduced during workflow runs. This information is often represented through provenance graphs, which can be used by scientists to better understand, reproduce, and verify scientific results. However, while most systems record and store data and process dependencies, few provide easy-to-use and efficient approaches for accessing and querying provenance information. Instead, users formulate provenance graph queries directly against physical data representations (e.g., relational, XML, or RDF), leading to queries that are difficult to express and expensive to evaluate. We address these problems through a high-level query language tailored for expressing provenance graph queries. The language is based on a general model of provenance supporting scientific workflows that process XML data and employ update semantics. Query constructs are provided for querying both structure and lineage information. Unlike other languages that return sets of nodes as answers, our query language is closed, i.e., answers to lineage queries are sets of lineage dependencies (edges) allowing answers to be further queried. We provide a formal semantics for the language and present novel techniques for efficiently evaluating lineage queries. Experimental results on real and synthetic provenance traces demonstrate that our lineage based optimizations outperform an in-memory and standard database implementation by orders of magnitude. We also show that our strategies are feasible and can significantly reduce both provenance storage size and query execution time when compared with standard approaches.

1. INTRODUCTION

Scientific results are often based on complex data analysis pipelines that integrate multiple domain-specific applications [14]. Automating the use of these applications is frequently performed using traditional scripting languages, and more recently, through scientific workflow systems (e.g., [20, 27, 9]). An advantage of scientific workflow systems over traditional approaches is their ability to automatically record the provenance of intermediate and final data products generated during workflow execution. This provenance information generally consists of data and process dependencies introduced during a workflow run, and is crucial for enabling scientists to more easily understand, reproduce, and verify scientific results [13].

Scientific workflow provenance is typically represented using data and process *dependency* (i.e., *causal*) *graphs* [19]. The ability to effectively store and query large numbers of dependency graphs remains a significant challenge in managing provenance information [13], since provenance graphs are typically heterogeneous (i.e., they do not share a common "schema") and each such graph may require considerable storage space. In particular, provenance information may be many times larger than the workflow and input data itself [11], workflows are often executed multiple times over different data sets and parameter settings, and most scientific research projects consist of many distinct workflows [4, 2]. To help address these challenges, a number of approaches have recently been proposed for efficiently representing and storing provenance dependency graphs [11, 16, 2, 5].

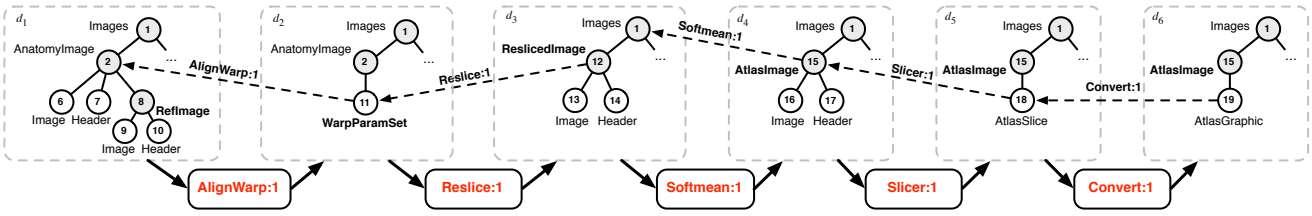
Approaches for querying stored provenance information, however, are largely still based on underlying physical data representations [13] (e.g., relational, XML, or RDF schemas), where users express provenance queries through corresponding query languages (i.e., SQL, XQuery, or SPARQL). Typical provenance queries (e.g., see [24]) are exploratory and involve finding some or all of the data and process dependencies that led to the creation of one or more data products. Posed over dependency graphs, these queries require the computation of transitive closures as well as applying selection conditions on corresponding lineage paths. For most users, expressing these queries against the physical schemas used to represent provenance information requires considerable expertise and is cumbersome even for simple queries [13]. The complexity of these queries also presents a number of challenges for efficient query evaluation [15].

In this paper we present a high-level *query language for provenance* (QLP; pronounced "clip") and novel evaluation techniques to address these challenges. Our query language provides basic constructs that are tailored to querying provenance information, which can help make common provenance queries easier to express for non-experts. In addition, unlike other standard languages that return sets of nodes (e.g., [10, 17, 29, 12, 6]), QLP is closed under lineage relationships. That is, answers to lineage queries are sets of lineage dependency *edges* forming provenance subgraphs. This approach simplifies the expression of complex queries, better supports provenance view definitions and graph visualization [13, 7], and leads to query optimizations described in this paper.

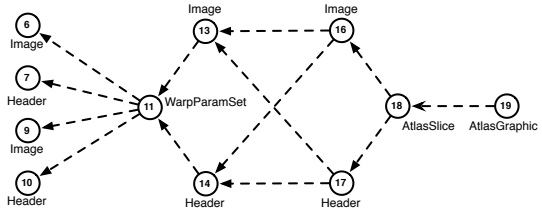
QLP employs a general model of provenance to support a wide

EDBT 2010, March 22–26, 2010, Lausanne, Switzerland.

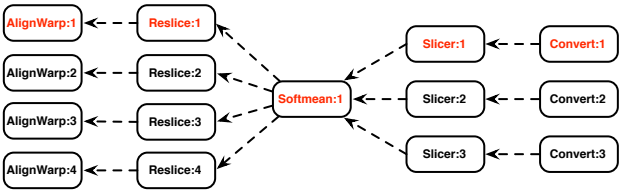
(a). The first provenance challenge fMRI workflow graph



(b). Trace $T = <V, F, L>$ with fine-grained node dependencies L and flow relations F for the first invocation of each actor



(c). Fine-grained data dependency view on lineage graph L



(d). Complete invocation dependency view on flow graph F

Figure 1: (a) Example XML-based workflow implementing the fMRI image analysis of the first provenance challenge; (b) The trace showing the first invocations of each actor for a typical run; (c) The implied fine-grain data dependency graph for the data items in (b); and (d) The implied invocation dependency graph for the run, with the first invocations of each actor shown in red.

range of scientific workflow systems. Most existing approaches for representing provenance do not consider workflow computation models that work over structured data, including XML. These standard provenance representation schemes (e.g., [19, 25, 17, 5, 6] among others) largely assume that workflow models are based on *transformation semantics*, where each workflow step consumes all input data and produces entirely new output data. Alternatively, workflow models that work over structured data (e.g., [7, 23, 26, 27]) often employ *update semantics*, where only a portion of an incoming XML structure is modified by each workflow step. Using update semantics can lead to a number of benefits for workflow design and reuse [3]. However, standard provenance approaches often cannot represent dependency relationships correctly or efficiently for XML-structured data [2, 23]. The model of provenance used by QLP extends conventional approaches by explicitly supporting workflow steps that process XML data and employ update semantics [3], and QLP includes query constructs for accessing both the structure and lineage of data items. More generally, QLP can be used in a wide range of situations where data is structured into nested collections and dependencies are defined among data nodes.

Contributions. This paper extends our prior work on efficiently storing [2] and querying [3] scientific workflow provenance over standard relational database technology. The main contributions include: (i) a formal semantics for QLP constructs introduced in [3]; (ii) techniques for evaluating QLP constructs; (iii) query optimization strategies that leverage the lineage-graph reduction approaches presented in [2]; (iv) novel algorithms for evaluating lineage queries between sets of nodes of increasing path length; and (v) experimental results verifying the effectiveness of our optimization techniques using real-life and synthetic provenance traces. In addition, we show that it is possible to simultaneously reduce the amount of storage required to represent scientific workflow provenance without negatively affecting query performance using our techniques. Our results show that unlike using standard approaches (which are often based on in-memory implementations, e.g., [29, 15, 21]), answering QLP queries using our optimization techiques over a relational database system is both feasible and scales with the size of provenance information and query complexity. While targeted at provenance applications, our optimizations can also be used in more general settings to efficiently answer a broad range of path queries over labeled, acyclic digraphs.

Organization. This paper is organized as follows. Section 2 introduces our provenance model and provides an overview of QLP through examples. Section 3 gives a formal semantics for QLP query constructs. Section 4 then describes different approaches for evaluating QLP lineage queries against various strategies, including our proposed techniques. Section 5 describes our experimental evaluation of the QLP optimization techniques presented in Section 4, considering both real and synthetic scientific workflow provenance traces. Section 6 discusses related work, and we conclude in Section 7.

2. PROVENANCE MODEL AND QLP

Consider the workflow in Fig. 1(a) showing a straightforward XML-based implementation of the fMRI image processing pipeline used in the First Provenance Challenge [19]. We refer to steps in the workflow as *actors* that are *invoked* over input data supplied by previous steps.[1] This workflow takes a set of anatomy images representing 3D brain scans and a reference image, and applies the actors in Fig. 1(a) as follows. (1) AlignWarp is invoked over each anatomy image to produce a set of "warping" parameters; (2) Reslice is invoked over each set of warping parameters to transform the associated anatomy image; (3) Softmean averages the transformed images into an atlas image; (4) Slicer produces three different 2D slices of the atlas; and (5) Convert is invoked over each 2D slice to create a graphical image.

[1] In general, we also consider more complex workflow graphs involving branching, merging, and loops, as in [20, 2, 7].

In this implementation of the workflow, each invocation of an actor receives an XML structure, performs an update on a portion of that structure, and then sends the updated version of the structure to downstream actors (see Fig. 1b). Here we assume that each XML structure denotes an unranked, labeled ordered tree representing workflow data products, each tree node is assigned a unique identifier, and tree nodes represent either *collection tokens* or *data tokens* (which wrap complex objects or reference external data, e.g., stored within a file). A collection token may be an internal node (for non-empty collections) or a leaf node (for empty collections), whereas data tokens are leaf nodes only.

Fig. 1(b) shows the first invocation of each actor for a typical run of the workflow. The invocation of the AlignWarp actor (shown as *AlignWarp:1*) modifies the first AnatomyImage collection (node 2), and replaces its contents with a WarpParamSet data token (node 11). Similarly, the invocation of the Reslice actor uses this WarpParamSet to generate a new Image and Header data token (nodes 13 and 14, respectively). As shown, explict "fine-grained" data dependencies are represented as part of the provenance of a run for cases when only a portion of an input data structure d is modified by an invocation. For example, the dashed arrow from node 11 to node 2 in Fig. 1(b) states that the WarpParamSet was created from the AnatomyImage collection by the first invocation of AlignWarp. Note that implicitly, node 11 depends on each of the descendents of node 2 (which includes nodes 6-10 in the figure). Similarly, each descendent of a collection implicitly inherits the dependencies of its ancestors (unless otherwise given). In our example, node 13 is a descendent of node 12 (a ReslicedImage collection), and thus implicitly depends on node 11. Taken together, Fig. 1(b) denotes a portion of the *trace* for a run of Fig. 1(a); in particular, this trace shows only the information associated with the first invocation of each workflow actor.

Traces can be used to derive conventional data and process dependency graphs (as views), as shown in Fig. 1(c) and 1(d), respectively. Here, the data dependency graph only shows dependencies for data nodes in Fig. 1(b), whereas the invocation dependency graph shows the complete set of invocations, assuming that four anatomy images were supplied to the workflow and three slices were created. Note that while the trace can be used to infer the data and invocation dependencies, the full trace cannot be reconstructed from these two graphs alone.

QLP queries are posed against provenance traces using the constructs outlined in Table 1. These constructs were chosen based on the common types of provenance queries identified in the literature [22, 13, 24, 8] (also see [3]). Different QLP constructs are used to query over distinct *dimensions* of the trace (see Fig. 1) representing: (i) *lineage relations* among nodes and invocations; (ii) *flow relations* among input and output data structures of invocations; and (iii) *structural relations* among nodes within and across data structures. We describe each of these dimensions below, using Fig. 1 as an example.

Queries over Lineage Relations. QLP lineage queries are closed under lineage relations such that a lineage query takes as input a set of lineage relations (edges) L and returns a subset of these lineage edges as output. A lineage edge in L is of the form $\langle n_1, i, n_2 \rangle$ stating that a node n_1 was used to derive a node n_2 via invocation i. In this way L denotes the "derived" relation such that each edge in L^{-1} is a "dependency".[2] For example, consider a lineage edge $\langle 2, \text{AlignWarp:1}, 11 \rangle$ of Fig. 1(b) stating that node 2 was used by the first invocation of the AlignWarp actor to produce node 11 (i.e., node 11 *depends on* node 2). Sets of lineage relations define lineage graphs, and QLP lineage queries act as filters over these lineage relations. For example, consider the following QLP lineage queries over the trace of Fig. 1(b).

```
* derived 19                          (1)
6 derived *                          (2)
* through Slicer:1 derived *          (3)
```

These queries return (1) lineage relations denoting the set of paths starting from any node and ending at node 19, (2) lineage relations denoting the set of paths starting at node 6 and ending at any node, and (3) lineage relations denoting the set of paths that go through the first invocation of the Slicer actor. QLP supports both a descriptive form (used above) and a shorthand notation. Using the shorthand notation, the above queries can be equivalently expressed as: '*..19', '6..*', and '*..#Slicer:1..*' (or simply '*..#Slicer:1' or '#Slicer:1..*'). Nodes and invocations form *steps* within lineage queries (generalized to XPath expressions and actor names below), and lineage queries consist of two or more steps.

Queries 1-3 select lineage paths of length one or greater (referred to as *transitive paths*). Although not shown in Table 1, QLP also supports queries that select lineage paths having length one (i.e., *immediate paths*) using the '.' operator, or in the descriptive form, using the operators 1_derived (for nodes) and 1_through (for invocations). Immediate and transitive path operators can be combined in QLP. For example, the following query returns the lineage relations defining dependency paths that start at an input node of the first invocation of the AlignWarp actor.

```
* 1_through AlignWarp:1 derived *     (4)
```

Finally, lineage queries can be chained together, e.g., the following queries

```
2 derived 12 derived 15                          (5)
2 through Reslice:1 through Slicer:1 1_derived *  (6)
```

return (5) lineage relations denoting paths that start at node 2 and end at node 15 while passing through node 12, and (6) lineage relations that start at node 2 and end at an output node of the first invocation of Slicer while passing through the first invocation of Reslice.

Queries over Flow Relations. QLP also allows lineage graphs to be filtered based on specific versions (or occurrences) of nodes within a trace using the @in and @out operators. For example, the following queries

```
* @in derived 19                      (7)
6 derived * @out                     (8)
* @in Slicer:1 derived *              (9)
15 @in Slicer:1 derived *            (10)
15 @out Slicer:1 derived *           (11)
```

return (7) lineage relations denoting paths that start at a node in the input data structure provided to the workflow run and end at node 19, (8) lineage relations denoting paths that start at node 6 and end at a node in an output structure of the workflow run, (9) lineage relations denoting paths that start at a node in an input structure of the first invocation of Slicer, (10) lineage relations denoting paths that start at the occurrence of node 15 in the input of the first invocation of Slicer, and (11) lineage relations denoting paths that start at the occurrence of node 15 in the output of the first invocation of Slicer. Note that queries 1 and 7 (and similarly, queries 2 and 8) are not equivalent for all traces. In particular, query 7 only returns lineage graphs with paths starting at an input node of the workflow run, whereas query 1 may contain paths starting at an intermediate node (e.g., a node created by an invocation, but without data depen-

[2]We draw lineage edges as "dependencies" (see Fig. 1) in which edges are labeled by their corresponding invocations.

Table 1: Summary of basic QLP constructs and corresponding descriptive notations

Construct	*Descriptive Form*	*Result*
Node and invocation expressions		
n, x, *	n, x, *	Node expressions e_n as a single node n, XPath expression x, or set of trace nodes *.
#i, #a	i, a	Invocation expressions e_i as an invocation i or actor a (denoting the set of a invocations).
e_n @in e_i	e_n @in e_i	Nodes of e_n input to invocations of e_i. If e_i is not given, then the nodes of e_n input to the workflow run.
e_n @out e_i	e_n @out e_i	Nodes of e_n output by invocations of e_i. If e_i is not given, then the nodes of e_n output by the workflow run.
Lineage-preserving path queries (examples)		
*..e_n	* derived e_n	The lineage graph for nodes in e_n.
e_n ..*	e_n derived *	The lineage graph for all nodes derived from nodes in e_n.
e_{n_1} ..e_{n_2}	e_{n_1} derived e_{n_2}	The lineage graph containing all paths from nodes in e_{n_1} to nodes in e_{n_2}.
e_{n_1} ..e_i ..e_{n_2}	e_{n_1} through e_i derived e_{n_2}	The lineage graph containing all paths from nodes in e_{n_1} to nodes in e_{n_2} that pass through an invocation in e_i.
Functions over path queries		
exists(p)	exists(p)	True if the trace contains a path defined by path query p.
invocations(p)	invocations(p)	The invocations of the lineage graph returned by path query p.
actors(p)	actors(p)	The actors of invocations of the lineage graph returned by path query p.
nodes(p)	nodes(p)	The nodes of the lineage graph returned by path query p.
input(p)	input(p)	The source nodes of the lineage graph returned by path query p.
output(p)	output(p)	The sink nodes of the lineage graph returned by path query p.

dencies). Also note that for the trace of Fig. 1(b), query 11 returns an empty set of lineage relations since node 15 is not a dependency of another node after the first invocation of Slicer.

Queries over Structural Relations. In addition to specific node identifiers, QLP queries can also contain XPath expressions for accessing nodes based on their type (i.e., tag name) and parent-child relationships. For example, consider the following queries.

* derived //AtlasImage//* (12)

/AnatomyImage[@modality="speech"]//* derived * (13)

These queries return (12) lineage relations denoting paths that end at a descendent node of an AtlasImage collection, and (13) lineage relations denoting paths that start at a descendent node of an AnatomyImage collection having the value "speech" for the modality metadata attribute. QLP also allows actor names to be used in place of specific invocations. In this case, the actor name denotes the set of invocations of the actor within the trace, returning lineage relations denoting paths that pass through one of the actor's invocations. Similar to attributes in XPath, we also allow invocation expressions to be selected based on their parameters, e.g., the expression 'Slicer[@x="0.5"]' selects invocations of Slicer in which the parameter x is set to "0.5".

Queries over Each Dimension. Each of the above dimensions can be combined into a single query. For example, the following query returns the set of lineage relations denoting paths that end at a descendent node of an AtlasImage collection output by a Slicer invocation.

* derived //AtlasImage//* @out Slicer (14)

Combined queries can be (naively) evaluated by (i) obtaining the structures resulting from @in and @out version operators, (ii) applying XPath expressions to these structures, and (iii) applying lineage queries to the resulting nodes. For example, when applied to the portion of the trace shown in Fig. 1(b), query 14 is evaluated by: (i) obtaining the output structure of the Slicer invocation; (ii) executing the XPath query '//AtlasImage//*' over the structure obtained in (i), returning nodes 16–19; and (iii) issuing a separate lineage query for each node, i.e., '* derived 16', '* derived 17', '* derived 18', and '* derived 19', where the answer contains the unique set of resulting lineage relations.

Additional Functions over Lineage Relations. Table 1 gives a number of additional functions that can be applied to the results of QLP lineage queries. The exists function determines whether a trace contains a given path; invocations and actors return for a set of lineage relations the invocations and actors, respectively; nodes returns the nodes contained in a set of lineage relations; and input and output return the source and sink nodes in a set of lineage relations, respectively.

The following section provides a more detailed and formal treatment of the constructs presented here, and QLP evaluation techniques are presented in Section 4.

3. QLP SYNTAX, AND SEMANTICS

Provenance model. We consider the following QLP provenance model. A *workflow trace* $T = \langle V, F, L \rangle$ consists of:

(i) a set of vertices $V = D \cup I$, where D is a set of XML data structures defined over nodes N, and I is a set of invocations over actors A;

(ii) a set of *flow edges* $F = F_{in} \cup F_{out}$, where $F_{in} \subseteq D \times I$ and $F_{out} \subseteq I \times D$ denote invocation inputs and outputs, respectively; and

(iii) a set of *lineage edges* $L \subseteq N \times I \times N$ denoting an acyclic digraph, where $\langle n_1, i, n_2 \rangle \in L$ states that invocation i used n_1 to create n_2.

An XML data structure $d \in D$ consists of nodes $n \in N$ such that nodes(d) are the nodes of d. A structure d is similar to a snapshot (or version) of an overall XML document denoting the output and/or input of each workflow step, e.g., Fig. 1(b) contains six such data structures d_1–d_6. We write $A(i)$ to denote the actor associated with an invocation $i \in I$ and $I(a)$ to denote the set of invocations associated with an actor $a \in A$. The input and output structures of a trace T (i.e., of the corresponding workflow run) are defined as:

$$\begin{aligned} \mathsf{in}(T) &= \{d \in D \mid \neg\exists i \in I : \langle i, d \rangle \in F_{out}\} \\ \mathsf{out}(T) &= \{d \in D \mid \neg\exists i \in I : \langle d, i \rangle \in F_{in}\}. \end{aligned}$$

QLP Syntax. QLP (shorthand) path expressions p are built from the following grammar.

$$\begin{aligned} p &::= s.s \mid s..s \mid s.p \mid s..p \\ s &::= e_n \mid e_n\ q \mid e_i \\ e_n &::= n \mid x \mid * \\ e_i &::= \#a \mid \#i \\ q &::= \text{@in} \mid \text{@out} \mid \text{@in}\ e_i \mid \text{@out}\ e_i \end{aligned}$$

A path p is composed of two or more steps s. A step is either a node expression e_n or an invocation expression e_i. A node expression

$$
\begin{aligned}
[\![n]\!] &:= \{n\} \\
[\![x]\!] &:= \{n \mid d \in D, n \in x(d)\} \\
[\![*]\!] &:= \{n \in N\} \\
[\![\#a]\!] &:= \{i \in I(a)\} \\
[\![\#i]\!] &:= \{i\}. \\
[\![e_n \ @\mathsf{in}]\!] &:= \{n \in [\![e_n]\!] \mid d \in \mathsf{in}(T), n \in \mathsf{nodes}(d)\} \\
[\![e_n \ @\mathsf{out}]\!] &:= \{n \in [\![e_n]\!] \mid d \in \mathsf{out}(T), n \in \mathsf{nodes}(d)\} \\
[\![e_n \ @\mathsf{in} \ e_i]\!] &:= \{n \in [\![e_n]\!] \mid d \in D, i \in [\![e_i]\!], \langle d, i\rangle \in E_{in}, \\
&\qquad n \in \mathsf{nodes}(d)\} \\
[\![e_n \ @\mathsf{out} \ e_i]\!] &:= \{n \in [\![e_n]\!] \mid d \in D, i \in [\![e_i]\!], \langle i, d\rangle \in E_{out}, \\
&\qquad n \in \mathsf{nodes}(d)\}
\end{aligned}
$$

Figure 2: Semantics of step expressions $s(T)$.

$$
\begin{aligned}
[\![e_{n_1}.e_{n_2}]\!](L) &:= \{\langle n_1, i, n_2\rangle \in L \mid n_1 \in [\![e_{n_1}]\!], n_2 \in [\![e_{n_2}]\!]\} \\
[\![e_{n_1}.e_i]\!](L) &:= \{\langle n_1, i, n_2\rangle \in L \mid n_1 \in [\![e_{n_1}]\!], i \in [\![e_i]\!]\} \\
[\![e_i.e_{n_2}]\!](L) &:= \{\langle n_1, i, n_2\rangle \in L \mid i \in [\![e_i]\!], n_2 \in [\![e_{n_2}]\!]\} \\
[\![e_{i_1}.e_{i_2}]\!](L) &:= \{\langle n_1, i_1, n_2\rangle, \langle n_2, i_2, n_3\rangle \in L \mid i_1 \in [\![e_{i_1}]\!], i_2 \in [\![e_{i_2}]\!]\}
\end{aligned}
$$

Figure 3: Semantics of simple immediate path expressions $s_1.s_n(T,L)$.

can be either an XPath x, a wildcard *, or a single node identifier n. An invocation expression specifies either an actor $\#a$ denoting all invocations of a, or an invocation identifier $\#i$.[3] Node expressions are optionally qualified with either an @in or @out operator. A *simple* path consists of exactly two steps in which $s_1.s_2$ is referred to as an *immediate* simple path and $s_1..s_2$ a *transitive* simple path.

QLP Semantics. Let $T = (V,F,L)$ be a trace defined over nodes N, invocations I, and actors A. Each individual step s is defined as a function that maps traces T to sets of vertices such that $s(T)$ returns a subset of V, as shown in Fig. 2. For XPath expressions x and XML structures d, in the normal way, $x(d)$ returns those nodes in d satisfying the expression x.

We define QLP path expressions p as functions that take traces $T = (V,F,L_0)$ and lineage graphs $L \subseteq L_0$ and return the given trace together with a new lineage graph L_p. Specifically, if p is a path expression, $T = (V,F,L_0)$ is a trace, and L is a lineage graph, $p(T,L) = \langle T, L_p\rangle$ such that $L_p \subseteq L$. Simple immediate path expressions of the form $s_1.s_2$ for traces T and lineage graphs L are defined in Fig. 3. For convenience we generally omit T when writing steps (as in Fig. 2) and paths (as in Figs. 3, 4, and 5).

Before defining more complex path expressions, we first consider the exists operator in Fig. 4, which returns true if a given lineage graph contains a path p and false otherwise. Checking whether a path $s_1..s_2$ exists in L (i.e., the second definition in Fig. 4) employs recursion: a path exists if an immediate path exists between s_1 and s_2 or else if there is a node n such that an immediate path exists from s_1 to n and a transitive path exists from n to s_2.

The last two definitions in Fig. 4 consider the general case of paths of length $m > 2$. As shown, invocation expressions are treated as a special case since in general it is difficult to replace an invocation with a corresponding node (without introducing a number of additional conditions). For example, consider a lineage graph comprising of two edges $\langle n_1, i_1, n_2\rangle$ and $\langle n_2, i_2, n_3\rangle$, and the 3-step query $\mathsf{exists}(n_1..i_1..n_2)$. Replacing i_1 in the query with its input n_1 results in the two subqueries $\mathsf{exists}(n_1..n_1)$ and $\mathsf{exists}(n_1..n_2)$, whereas replacing i_1 with its output n_2 results in the subqueries $\mathsf{exists}(n_1..n_2)$ and $\mathsf{exists}(n_2..n_2)$, both of which consist of unsatisfiable subqueries of the form $\mathsf{exists}(n..n)$. This issue is addressed by the fourth definition in Fig. 4, which for this example first computes $n_1..n_2$ over L, and then checks if both $n_1..i_1$ and $i_1..n_2$ exist in the result (i.e., if i_1 can be reached from n_1, and n_2 can be reached from i_1). Note that for general paths from s_1 to s_m, after applying $s_1..s_m$, if it is possible to reach an invocation i from s_1, then trivially i falls on a path to s_m, and conversely, if it is possible to reach s_m from i, then i must trivially fall on a path from s_1.

Transitive path queries are defined in Fig. 5. Similar to Fig. 4, invocations in path expressions of length $m > 2$ are defined as a special case. Note also that in each definition of Fig. 5, we require that a given path exists prior to returning lineage relations. Without such a check, it is possible that edges forming incomplete paths could be returned.

Finally, we note that because QLP lineage queries return sets of dependency edges, more complex queries can be built from path expressions using standard set operations. For instance, given two QLP path expressions p_1 and p_2, it is possible to combine these into more complex queries using set intersection $p_1 \cap p_2$, union $p_1 \cup p_2$, and difference $p_1 - p_2$.

4. QLP EVALUATION TECHNIQUES

In this section we describe techniques for evaluating transitive path queries in QLP, i.e., queries that use the '..' operator, since these are often considerably more expensive to evaluate (e.g., see [16, 2]) than XPath queries or queries that simply select specific versions of structures within a trace (using @in and @out). The evaluation of transitive path queries is closely tied to how lineage relations are stored. Thus, the techniques proposed here consider different approaches for storing lineage relations and associated techniques for answering queries.

We consider path expressions p that take the form $s_1..s_2..s_3 \cdots s_m$ of length $m > 1$ such that for a set of lineage relations L, we select the set of paths in L satisfying p, and return these paths as a subset of the given lineage relations. To simplify the discussion, we assume that each step s_i in p can be evaluated to a set of nodes N_i. Thus, a path expression $p = s_1..s_2$ can be rewritten as $N_1..N_2$ denoting a set of subqueries such that the answer to p is comprised of the answers to each of the simpler subqueries $n_1..n_2$ for $n_1 \in N_1$ and $n_2 \in N_2$.

If a step s in p is an invocation expression, we construct the corresponding set of nodes as follows. First, we use $\mathsf{in}(s)$ and $\mathsf{out}(s)$ to denote the set of input and output nodes across invocations of s. Let $p = s_1..s_2$. If s_1 is an invocation expression and s_2 a node expression evaluating to N_2, we rewrite p as $\mathsf{in}(s_1)..(\mathsf{out}(s_1) \cup N_2)$. Similarly, if s_2 is also an invocation expression, we rewrite p as $\mathsf{in}(s_1)..\mathsf{out}(s_2)$. Finally, if s_1 is a node expression evaluating to N_1 and s_2 an invocation expression, we rewrite p as $(N_1 \cup \mathsf{in}(s_2))..\mathsf{out}(s_2)$. Rewriting lineage queries in this way can be easily extended to paths containing more than two steps.

We start by presenting different strategies (denoted I, ICP, $ICP(N)$, and $ICP(S)$) for storing lineage graphs and discuss their trade-offs in terms of storage and query efficiency. We then describe additional optimization techniques for queries involving paths containing more than 2 steps and for cases when steps evaluate to multiple nodes.

Immediate Lineage Edges (I). A common approach for storing lineage graphs is to store only the immediate edges in an edge table $\mathrm{Edge}(N_1, I, N_2)$. Evaluating path expressions in this case requires recursion or iteration over the edges of the graph. For example,

[3] As a convention, invocations are written `a:1`, denoting in this case the first invocation of actor `a`.

$$
\begin{aligned}
[\![\mathsf{exists}(s_1\,.\,s_2)]\!](L) &\equiv [\![s_1\,.\,s_2]\!](L) \neq \emptyset \\
[\![\mathsf{exists}(s_1\,..\,s_2)]\!](L) &\equiv [\![\mathsf{exists}(s_1\,.\,s_2)]\!](L) \vee (\exists n \in N : [\![\mathsf{exists}(s_1\,.\,n)]\!](L) \wedge [\![\mathsf{exists}(n\,..\,s_2)]\!](L)) \\
[\![\mathsf{exists}(s_1 \circ_1 e_n \circ_2 s_3 \cdots s_m)]\!](L) &\equiv \exists n \in [\![e_n]\!] : [\![\mathsf{exists}(s_1 \circ_1 n)]\!](L) \wedge [\![\mathsf{exists}(n \circ_2 s_3 \cdots s_m)]\!](L) \\
[\![\mathsf{exists}(s_1 \circ_1 e_i \circ_2 s_3 \cdots s_m)]\!](L) &\equiv \exists i \in [\![e_i]\!] : [\![\mathsf{exists}(s_1 \circ_1 i)]\!]([\![s_1\,..\,s_m]\!](L)) \wedge [\![\mathsf{exists}(i \circ_2 s_3 \cdots s_m)]\!]([\![s_1\,..\,s_m]\!](L))
\end{aligned}
$$

Figure 4: Semantics of exists (i.e., reachability) queries over path expressions $s_1 \circ_1 s_2 \circ_2 \cdots s_m$ for $m \geq 3$ and $\circ$ an immediate or transitive path.

$$
\begin{aligned}
[\![s_1\,..\,s_2]\!](L) &:= [\![s_1\,.\,s_2]\!](L) \cup \{l \mid n \in N, [\![\mathsf{exists}(s_1\,.\,n)]\!](L), [\![\mathsf{exists}(n\,..\,s_2)]\!](L), l \in [\![s_1\,.\,n]\!](L) \cup [\![n\,..\,s_2]\!](L)\} \\
[\![s_1 \circ_1 e_n \circ_2 s_3 \cdots s_m]\!](L) &:= \{l \mid n \in [\![e_n]\!], [\![\mathsf{exists}\, s_1 \circ_1 n \circ_2 s_3 \cdots s_m]\!](L), l \in [\![s_1 \circ_1 n]\!](L) \cup [\![n \circ_2 s_3 \cdots s_m]\!](L)\} \\
[\![s_1 \circ_1 e_i \circ_3 s_3 \cdots s_m]\!](L) &:= \{l \mid i \in [\![e_i]\!], [\![\mathsf{exists}\, s_1 \circ_1 i \circ_2 s_3 \cdots s_m]\!](L), l \in [\![s_1 \circ_1 i]\!]([\![s_1\,..\,s_m]\!](L)) \cup [\![i \circ_2 s_3 \cdots s_m]\!]([\![s_1\,..\,s_m]\!](L))\}
\end{aligned}
$$

Figure 5: Semantics of transitive path expressions.

the following Datalog program can be used to compute the set of lineage relations $\langle x, i, y\rangle$ between any two nodes N_1 and N_2.

$$
\begin{aligned}
\mathrm{Q}(N_1,N_2,N_1,I,N_2) &:- \mathrm{Edge}(N_1,I,N_2). \\
\mathrm{Q}(N_1,N_2,N_1,I,N) &:- \mathrm{Edge}(n_1,I,N), \mathrm{Path}(N,N_2). \\
\mathrm{Q}(N_1,N_2,X,I,Y) &:- \mathrm{Edge}(N_1,I,N), \mathrm{Q}(N,N_2,X,I,Y). \\
\mathrm{Path}(N_1,N_2) &:- \mathrm{Edge}(N_1,I,N_2). \\
\mathrm{Path}(N_1,N_2) &:- \mathrm{Path}(N_1,N), \mathrm{Edge}(N,I,N_2).
\end{aligned}
$$

In the above query, Path is the transitive closure of the Edge relation. Query Q computes lineage relations as path nodes are traversed by recursively performing a breadth-first search (using both *Path* and Q) .

Here, we propose a more efficient approach in which we (i) compute the set of nodes on paths starting at node n_1 and ending at node n_2, and then (ii) join the resulting path nodes with the Edge table to return the corresponding lineage edges. The following Datalog program implements this approach, which returns the same set of edges as the previous program. In general, we adopt this query approach when considering the *immediate (edge)* storage strategy, which we denote as storage strategy I.

$$
\begin{aligned}
Q_I(N_1,N_2,X,I,Y) &:- \mathrm{PathNode}(N_1,N_2,X), \\
&\quad\ \mathrm{PathNode}(N_1,N_2,Y), \mathrm{Edge}(X,I,Y). \\
\mathrm{PathNode}(N_1,N_2,N_1) &:- \mathrm{Edge}(N_1,I,N_2). \\
\mathrm{PathNode}(N_1,N_2,N_2) &:- \mathrm{Edge}(N_1,I,N_2). \\
\mathrm{PathNode}(N_1,N_2,N) &:- \mathrm{Path}(N_1,N), \mathrm{Path}(N,N_2). \\
\mathrm{Path}(N_1,N_2) &:- \mathrm{Edge}(N_1,I,N_2). \\
\mathrm{Path}(N_1,N_2) &:- \mathrm{Path}(N_1,N), \mathrm{Edge}(N,I,N_2).
\end{aligned}
$$

Note that this approach has a single recursive rule (Path) whereas the previous approach has two recursive rules (Path and Q).

Immediate Edges and Dependency Closure (*IC*). The recursion in the previous approach can be removed by materializing the Path relation. Thus, this strategy (denoted *IC*) stores both the immediate edges in an edge table $\mathrm{Edge}(N_1,I,N_2)$ and the transitive closure over dependency nodes $\mathrm{Path}(N_1,N_2)$. To compute the set of nodes on lineage paths (PathNode), this approach must perform an expensive self-join on a potentially large Path table. In addition, to return a set of lineage relations, a join must still be performed between PathNode and the Edge table. Note that this approach increases storage size by materializing Path (at a cost of $O(n^2)$) to reduce query time by eliminating recursion.

Immediate Edges and Closure via Pointers (*ICP*). To address the issue of performing a self-join on large, materialized Path tables, we employ a "pointer-based" strategy (denoted here as *ICP*) that partitions the Path table into three smaller tables (based on reduction techniques) where the original Path table can be obtained by joining these smaller tables together. This pointer-based storage strategy is discussed in our earlier work [2]. In particular, the Path table is partioned into the following three tables (see Fig. 6)

- $\mathrm{Node}(N_2, I, P_{dep}, P_{depc})$
- $\mathrm{DepV}(P_{dep}, N_1)$
- $\mathrm{DepcV}(P_{depc}, P_{dep})$

where P_{dep} is a pointer to the set of immediate dependencies of n_2; and P_{depc} is a pointer to a set of immediate dependency pointers P_{dep}, representing the transitive dependency closure of n_2. Using this approach, the lineage graph shown in Fig. 6(a) is reduced to the graph in Fig. 6(b).

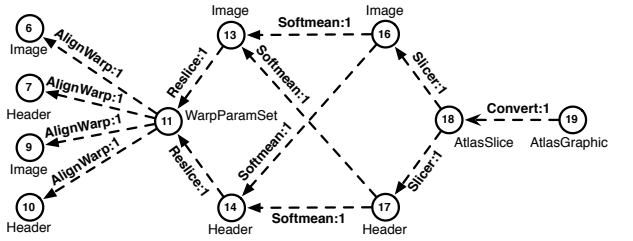
The basic idea of the approach is to use pointers to store a single copy of shared sets of dependency nodes. For instance, in Fig. 6(a), the dependency set for node 16 is $\{13,14\}$ and the dependency set for node 17 is also $\{13,14\}$. Instead of storing multiple copies of the same dependency set, a pointer &9 is used to refer to the dependency set $\{13,14\}$ in the DepV relation, and nodes 16 and 17 refer to pointer &9 in the Node relation. In addition, instead of storing the transitive closure between dependency nodes, DepcV stores the transitive closure of the immediate pointers, e.g., as shown by the dashed lines in Fig. 6(b). For instance, the transitive dependency closure of node 16 is the set of nodes $\{6,7,9,10,11,13,14\}$, whereas in the pointer-based representation, node 16 has the transitive dependency pointer $\&9'$ that refers to the transitive dependency (pointer) set $\{\&1,\&5,\&9\}$ in the DepcV relation.

The following rules can be used to reconstruct a node-based lineage graph from a pointer-based (reduced) lineage graph.

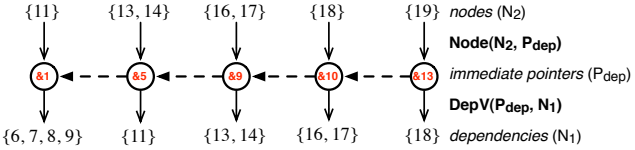
$$
\begin{aligned}
\mathrm{Edge}(N_1,I,N_2) &:- \mathrm{Node}(N_2,I,P_{dep},P_{depc}), \mathrm{DepV}(P_{dep},N_1). \\
\mathrm{Path}(N_1,N_2) &:- \mathrm{Node}(N_2,I,P_{dep},P_{depc}), \mathrm{DepcV}(P_{depc},P_{dep}), \\
&\quad\ \mathrm{DepV}(P_{dep},N_1).
\end{aligned}
$$

As described in [2], both *DepV* and *DepcV* are further reduced by factoring out common subsets of dependency sets. In this way, *DepV* and *DepcV* are simple views defined over the further reduced tables.

Note that these Edge and Path queries can be used with PathNode defined above to answer QLP path expressions of the form



(a). Node-based lineage graph



(b). Pointer-based (reduced) lineage graph for (a)

Figure 6: Lineage graph with corresponding pointer-based representations.

Algorithm 1 Evaluating single node-based path expressions (ICP)

Input: $p = n_1 .. n_2 .. n_3 \cdots n_m$
Output: Set of lineage relations

1: **for** $i \leq m-1$ **do**
2: **if** not $exists(n_i .. n_{i+1})$ **then**
3: **return** $\emptyset$ /* no lineage path for p*/
4: **end if**
5: **end for**
6: $N_p = \emptyset$
7: **for** $i \leq m-1$ **do**
8: $N_p = N_p \cup \{n \mid \text{PathNode}(n_i, n_{i+1}, n)\}$
9: **end for**
10: return $\{\langle x,i,y\rangle \mid x \in N_p, y \in N_p, Edge(x,i,y)\}$ /* lineage edge */

$n_1 .. n_2$. While computing the PathNode relation is more efficient in the pointer-based approach (since we avoid self-joins over the materialized Path table), it still requires a number of joins over intermediate relations (i.e., DepV, DepcV, Path, and PathNode). To more efficiently evaluate path expressions, we (i) temporarily materialize the views DepV and DepcV (which together contain fewer overall tuples than Path, as shown in Fig. 6); (ii) evaluate and materialize the queries $\text{Path}(N_1, N)$ and $\text{Path}(N, N_2)$; (iii) use these materialized Path queries to evaluate and materialize the query $\text{PathNode}(N_1, N_2, N)$; and (iv) use the materialized PathNode query to answer $\text{Q}(N_1, N_2, X, I, Y)$, returning the set of lineage edges $\langle x,i,y\rangle$.

Evaluating Simple Reachability Queries. To answer reachability queries between two nodes n_1 and n_2, i.e., $\text{exists}(n_1 .. n_2)$, we simply evaluate the query $\text{Path}(n_1, n_2)$.

Evaluating Single Node-Based Path Expressions. We evaluate general path expressions $p = n_1 .. n_2 .. n_3 \cdots n_{m-1} .. n_m$ for $m > 2$ using ICP by transforming the expression into a set of simple path expressions $n_i .. n_{i+1}$ (for $1 \leq i \leq m$). If each simple path is reachable, then we find the set of nodes for each simple path, and compute the set of edges over these nodes (see Algorithm 1).

Naive Evaluation of Set-Based Path Expressions ($ICP(N)$). A straighforward approach for evaluating set-based path expressions $p = N_1 .. N_2 \cdots N_m$ for N_i a set of nodes, is to rewrite p into multiple node-based path expressions $n_1 .. n_2 \cdots n_m$ for each $n_i \in N_i$. Each of these node-based path expressions are evaluated in a similar way as in Algorithm 1, i.e., for each node-based path expression we add the corresponding set of nodes returned to N_p and then compute the set of edges as in step 10 (i.e., computing edges is deferred until each of the node-based expressions is computed). Note however, that in this approach the number of node-based path expressions that must be computed from p is $|N_1| \times |N_2| \times \cdots \times |N_m|$. This node-based approach for evaluting path expressions is referred to as $ICP(N)$.

Algorithm 2 Efficiently evaluating set-based path expressions ($ICP(S)$)

Input: $p = N_1 .. N_2 .. N_3 \cdots N_m$
Output: Set of lineage relations

1: **for** $i \leq m$ **do**
2: $N_{F_i} = \{n \mid \text{Path}(n_i, n), n_i \in N_i\}$ /* forward lineage nodes */
3: $N_{B_i} = \{n \mid \text{Path}(n, n_i), n_i \in N_i\}$ /* backward lineage nodes */
4: **end for**
5: **for** $i \leq m$ **do**
6: $PN_i = N_i$
7: **for** $j \leq i-1$ **do**
8: $PN_i = PN_i \cap N_{F_j}$
9: **end for**
10: **for** $i+1 \leq j \leq m$ **do**
11: $PN_i = PN_i \cap N_{B_j}$ /* pruned set */
12: **end for**
13: **if** $(PN_i == \emptyset)$ **then**
14: **return** $\emptyset$ /* no lineage path for p*/
15: **end if**
16: **end for**
17: **for** $i \leq m$ **do**
18: $PN_{F_i} = \{n \mid \text{Path}(n_i, n), n_i \in PN_i\}$
19: $PN_{B_i} = \{n \mid \text{Path}(n, n_i), n_i \in PN_i\}$
20: **end for**
21: $N_p = \emptyset$
22: **for** $i \leq m-1$ **do**
23: $N_p = N_p \cup (PN_{F_i} \cap PN_{B_{i+1}})$
24: **end for**
25: return $\{\langle x,i,y\rangle \mid x \in N_p, y \in N_p, Edge(x,i,y)\}$ /* lineage edge */

Efficient Evaluation of Set-Based Path Expressions ($ICP(S)$). To avoid the cost of computing a potentially large number of node-based path expressions, we propose a more efficient approach that directly computes set-based path expressions (referred to as $ICP(S)$). For simple paths $N_1 .. N_2$, we first evalute $N_1 .. *$ as follows: (i) compute the set of pointers P_{dep} for the set of nodes N_1 from the DepV relation; (ii) from the set P_{dep} we select the set of transitive pointers P_{depc} from DepcV; (iii) from Node relation we select all nodes N_F (i.e., the "forward" lineage nodes) that have $p_{depc} \in P_{depc}$; and (iv) we add only those nodes from N_1 to the nodes obtained in (iii) that have a P_{dep} associated with them. We then use a similar approach to evaluate the expression $* .. N_2$, resulting in a set of nodes N_B (the "backward" lineage nodes). The set of nodes N on the lineage path from nodes in N_1 to nodes in N_2 is $N_F \cap N_B$. Finally, the set of lineage edges is computed from N.

Given a path expression of the form $p = N_1 .. N_2 \cdots N_m$ it may be the case that not all the nodesin the set N_i share a lineage relationship with all the nodes in the other set. In $ICP(S)$, we prune each of the sets N giving a new set PN such that each node $n_i \in PN_i$ shares a dependency relationship with at least one node in all other sets, and vice versa. We rewrite p to $PN_1 .. PN_2 \cdots PN_m$ and evaluate each simple path $PN_i .. PN_{i+1}$ as in Algorithm 2. Lines 1–4 compute "forward" and "backward" lineage nodes for each set N_i. Lines 5–16 prune each set N_i giving $PN_i = (\cap_{j=1}^{j=i-1} N_{F_i}) \cap N_i \cap (\cap_{k=i+1}^{k=m} N_{B_i})$ such that all nodes in the pruned sets PN_i are reachable from at least one node in each of the other sets. Lines 17–20 compute "forward" and "backward" lineage nodes for pruned sets PN_i. Lines 21–24 evaluate lineage nodes N_p for path expressions over pruned sets.

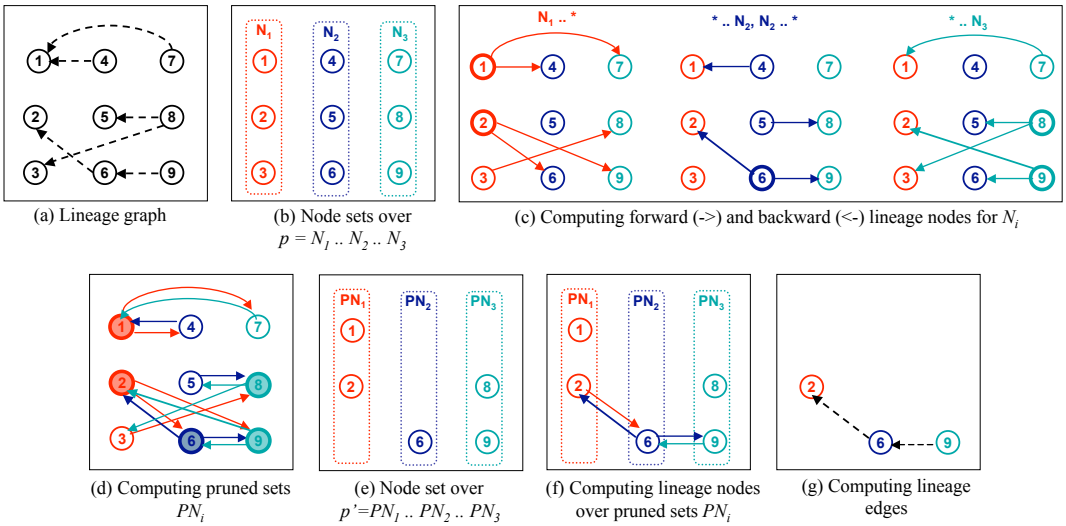


Figure 7: Example execution of set-based path expressions using Algorithm 2 for $p = N_1..N_2..N_3$: (a) the inital lineage graph where $N_1 = \{1,2,3\}$, $N_2 = \{4,5,6\}$ and $N_3 = \{7,8,9\}$; (b) the sets of nodes corresponding to N_1, N_2, and N_3; (c) the "forward" and "backward" lineage nodes for each N_i; (d) the pruned sets N_i such that all nodes in PN_i are reachable from at least one node in all other sets; (e) the pruned sets $p' = PN_1..PN_2..PN_3$; (f) the lineage nodes over pruned sets $N_p = nodes(PN_1..PN_2..PN_3) = \{2,6,9\}$; and (g) the lineage edges $\langle 2,\_,6\rangle$ and $\langle 6,\_,9\rangle$ returned as a result of the lineage nodes $\{2,6,9\}$.

Finally, line 25 computes lineage edges from the lineage nodes.

To help see how this approach works, consider a QLP path expression query $p = N_1..N_2..N_3$ for the lineage graph shown in Fig. 7(a), where $N_1 = \{1,2,3\}$ (red color), $N_2 = \{4,5,6\}$ (blue color), and $N_3 = \{7,8,9\}$ (green color). Fig. 7(c–g) shows the various stages of Algorithm 2 for evaluating set-based path expressions. Fig. 7(c)) shows all those nodes that are reachable from the nodes in each sets N_i. Fig. 7(d) selects those nodes from sets N_i such that all those nodes are reachable from at least one node in all other sets. Fig. 7(e) shows the pruned sets PN_i, where $PN_1 = \{1,2\}$, $PN_2 = \{6\}$, and $N_3 = \{8,9\}$, such that each node in Pn_i is reachable from at least one node in other sets. Fig. 7(f) shows the nodes that lie on lineage path over the pruned sets. Finally, Fig. 7(g) shows the lineage edges $\langle 2,\_,6\rangle$ and $\langle 6,\_,9\rangle$ over the lineage nodes $\{2,6,9\}$.

Unlike in $ICP(N)$, which requires $|N_1| \times |N_2| \times \cdots \times |N_m|$ simple path expressions $(N_i..N_{i+1})$ to be computed, $ICP(S)$ requires only $2 * m$ simple path expressions to be computed.

5. EXPERIMENTAL RESULTS

Here we evaluate the efficiency and scalability of answering QLP queries over the storage strategies of Section 4 on both real and synthetic traces. Real traces were generated from existing workflows implemented within the Kepler scientific workflow system (using the extensions described in [7, 3]). Our experiments were performed using a 2.4GHz Intel Core 2 duo PC with 2 GB RAM and 120 GB of disk space. Each storage strategy used PostgreSQL to store provenance information, and our QLP parser was implemented in Java using JDBC to communicate with the provenance database.

We compare query response time and storage size using *synthetic traces* ranging from 100 to 6000 nodes, $5 * 10^2$ to 10^5 immediate dependencies, 10^3 to 10^8 transitive dependencies, and lineage paths of length 10 to 100, respectively. The synthetic traces were taken from [2], and represent typical lineage patterns of common scientific workflows [2, 7, 24]. Fig. 8(a) shows the complexity of dependencies (immediate and transitive) as the nodes in synthetic traces increase, and Fig. 8(b) shows the storage size of these traces under the different storage strategies. As shown, the pointer-based approach used to store immediate and transitive dependencies in a reduced form leads to considerably smaller storage size [2].

We also evaluated our approaches using the following *real traces* from scientific workflows implemented within Kepler: the *PTP*, *GBL*, *CGR*, and *PLC* workflows [7] use different approaches to infer phylogenetic trees from protein and morphological sequence data; the *PC1* workflow was used in the first provenance challenge [24] (and is similar to the example shown in Fig. 1); the *STP*, *STM*, and *CYC* workflows are used in characterizing microbial communities by clustering and identifying DNA sequences of 16S ribosomal RNA; the *WAT* workflow characterizes microbial populations by producing phylogenetic trees from a list of sequence libraries; and the *PC3* workflow was used within the third provenance challenge[4]. The dependency annotations of these traces range from 10^2 to 10^4 with $2 * 10^2$ to $2 * 10^4$ transitive dependency edges.

We consider the following QLP queries for evaluating query response time.

$$*..n \quad \text{(Q1)}$$
$$n_1..n_2 \quad \text{(Q2)}$$
$$n_1..n_2..n_3 \quad \text{(Q3)}$$
$$*..N \quad \text{(Q4)}$$
$$N_1..N_2 \quad \text{(Q5)}$$
$$N_1..N_2..N_3 \cdots N_m \quad \text{(Q6)}$$

These queries return (Q1) lineage relations denoting paths that lead to a node n (e.g., to return the full lineage of n); (Q2) lineage relations denoting paths starting at node n_1 and ending at node n_2; (Q3) lineage relations denoting paths starting at node n_1 and ending at node n_3 that pass through node n_2; (Q4) lineage relations denoting paths that lead to nodes in a set of nodes N; (Q5) lineage relations denoting paths starting at nodes in a set N_1 and ending at nodes in a set N_2; and (Q6) lineage relations denoting paths that satisfying path expression of varying length m (e.g., in our experiments, m

[4]see `http://twiki.ipaw.info/bin/view/Challenge/`

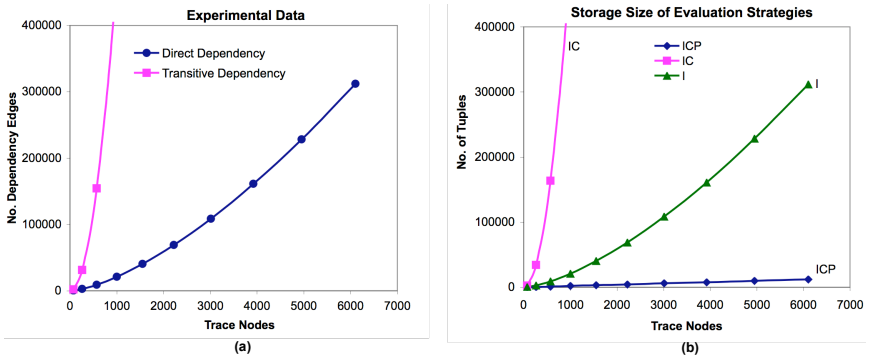


Figure 8: (a) shows dependency complexity of sample traces. (b) shows size for storing the sample traces in storage strategies.

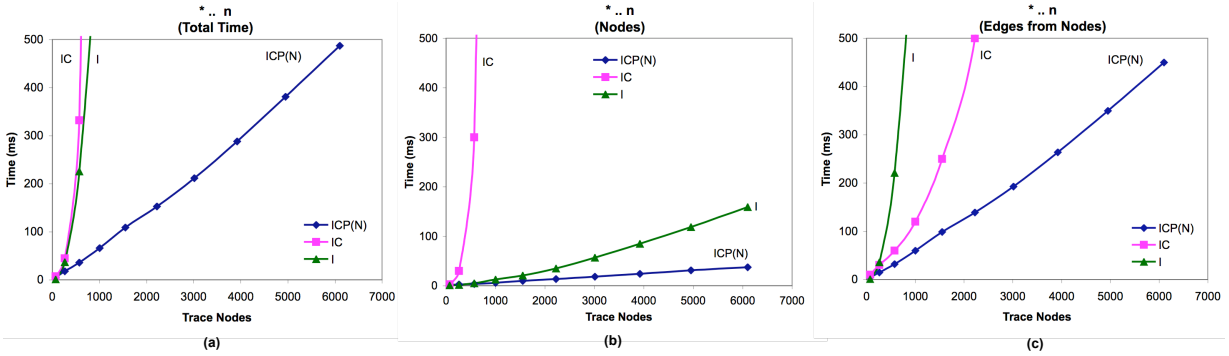


Figure 9: Evaluating * ..n over storage strategies.

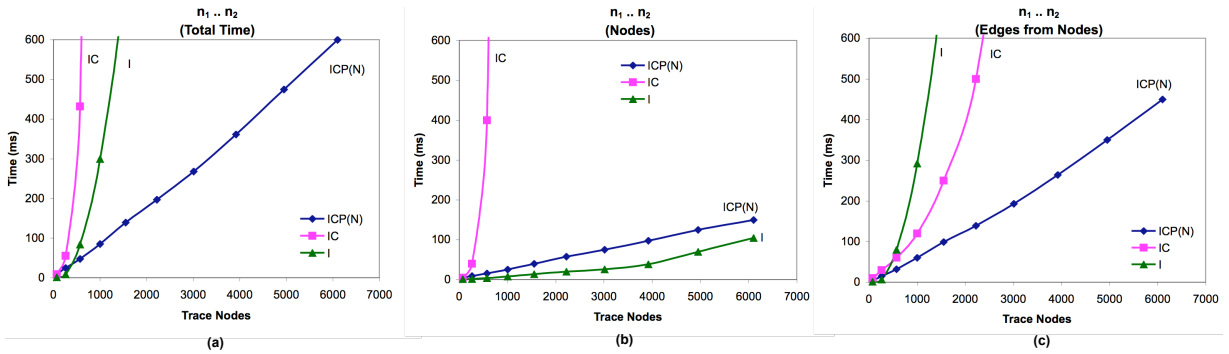


Figure 10: Evaluating n_1 ..n_2 over storage strategies.

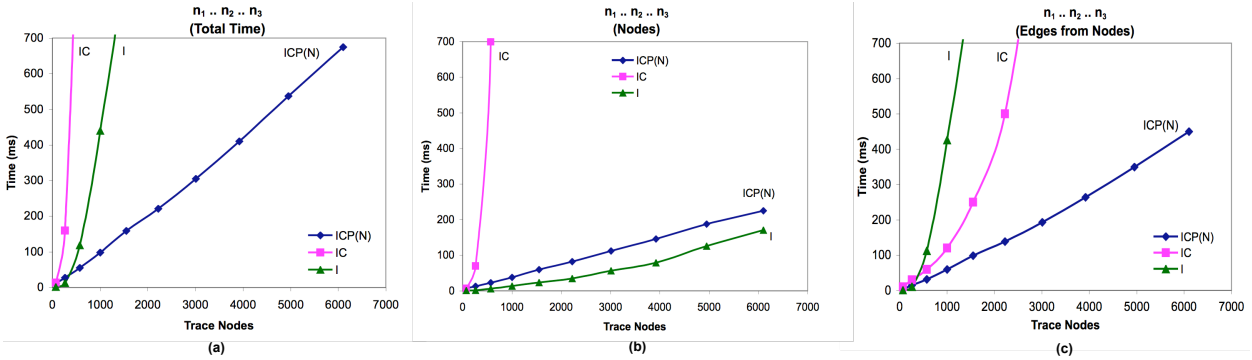


Figure 11: Evaluating n_1 ..n_2 ..n_3 over storage strategies.

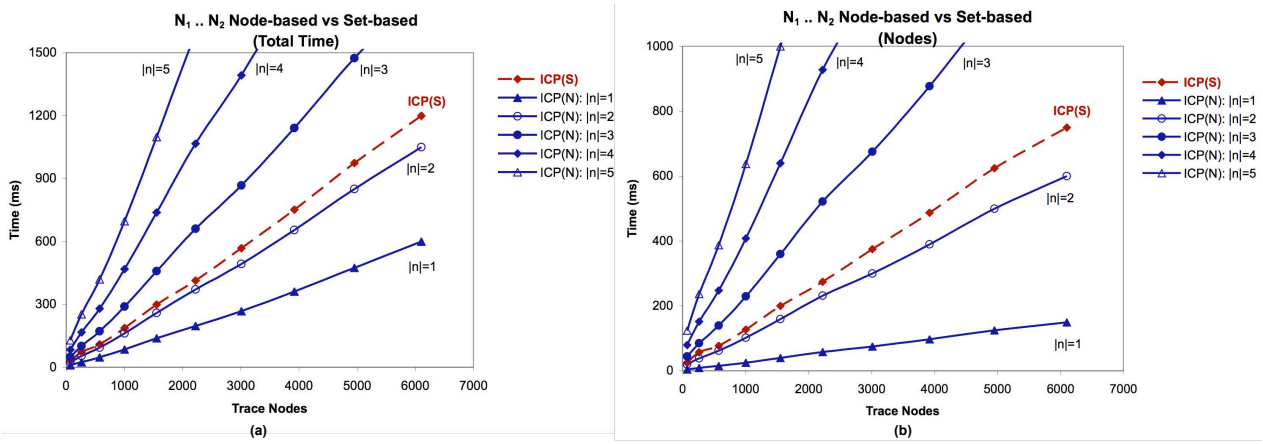


Figure 12: Comparing node-based $ICP(N)$ and set-based $ICP(S)$ approaches for evaluating N_1 ..N_2.

varies from 2 to 25).

These queries are evaluated over various storage strategies (*I*, *IC*, and *ICP*, described in Section 4). We implemented strategy *I* using XSB (a logic programming and deductive database system that supports in-memory queries[5]) whereas the implementation of *IC*, $ICP(N)$, and $ICP(S)$ uses PostgreSQL for storing and querying traces.

Paths with Single Node Identifiers. In queries Q1–Q3 each step evaluates to a single node identifier. Figs. 9–11 show the time to evaluate Q1, Q2, and Q3, respectively, over *I*, *IC*, and *ICP*. In each case, we show: (a) the total query execution time for computing lineage relations, (b) the portion of the total time used to compute the nodes that lie on the lineage path, and (c) the portion of the total time used to compute the lineage edges from the nodes returned in (b).

Fig. 9(a) shows that Q1 scales for $ICP(N)$ but does not scale for *IC* and *I*. *I* scales when returning set of nodes (Fig. 9(b)), but *I* does not scale for computing edges from these set of nodes (Fig. 9(c)). Similar results were observed for Q2 and Q3, which have more complex path expressions. We also observe that as path expressions increase in length, query time scales for $ICP(N)$ but not for *I* and *IC*. For example, for a trace containing 6000 nodes, Fig. 9 shows that $ICP(N)$ takes 500 ms, 600 ms, and 700 ms to evaluate Q1, Q2, and Q3, respectively, representing only a marginal increase in query response time as the length of paths increases.

Paths with Sets of Node Identifiers. In query Q5, each step evaluates to a set of node identifiers. Fig. 12 shows the time to evaluate Q5 over the storage strategies. Fig. 12 shows that when the node-based approach $ICP(N)$ is used to evaluate Q5, the query time is proportional to the product of the number of nodes in each path set. This is due to the number of node-based subqueries that $ICP(N)$ must evaluate. However, for the set-based approach $ICP(S)$, the query response time remains constant as the size of sets increase. As shown, $ICP(S)$ outperforms $ICP(N)$ when the number of nodes in each set is greater than 2.

Evaluating Path Expressions of Increasing Length. Fig. 13 shows that using the optimization techniques of $ICP(S)$, query response time scales linearly as the length of path expressions increase. In particular, we consider path expressions involving between 1 and 25 steps in Fig. 13. As shown, $ICP(S)$ can be used to efficiently and scalably evaluate complex QLP path expressions.

[5]see `http://xsb.sourceforge.net/`

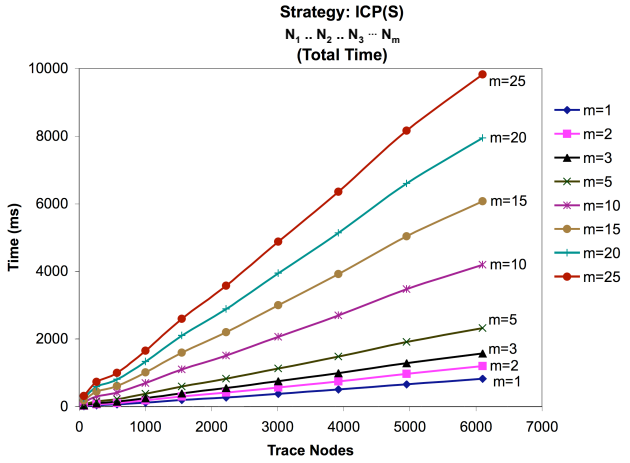


Figure 13: Evaluating N_1 ..N_2 ..$N_3 \cdots N_m$ using $ICP(S)$.

Storing and Querying Real Traces. Fig. 14(a) and (b) show the storage size for representing lineage graphs and transitive dependencies for the real traces under our storage strategies. Fig. 14(a) shows the storage size of "smaller" traces (trace nodes ranging from 80 to 200) and Fig. 14(b) shows the storage size of "bigger" traces (trace nodes ranging from 1000 to 10,000). Fig. 14(a) and Fig. 14(b) show that the space requirement for storing lineage relations in *ICP* is considerably less than in *I* and *IC*. Note that *I* stores only lineage edges, while *ICP* stores both lineage edges and transitive closure of dependency nodes using our reduction techniques, and in most of the cases (except PTP, PC1, and PC3), the storage size for *ICP* is less than that of *I* (implying that many nodes have similar dependencies). Also, although *ICP* stores the same information as *IC*, the storage size for *ICP* is less than that for *IC*.

Fig. 14(c) and (d) show the query time for evaluating Q4 and Q5 over real traces (both small and big) using *IC* and *ICP*. To consider complex queries, each step in the path expressions evaluate to all data nodes of the trace. As shown, path queries are evaluated using $ICP(S)$ in less than 10^2 ms, which is significantly less than using *IC* which can take up to 10^6 ms. This is because *IC* has to perform a self-join over the transitive closure table together with a join over the dependency table, both containing a large number of tuples, whereas $ICP(S)$ performs three joins over the reduced tables. If we

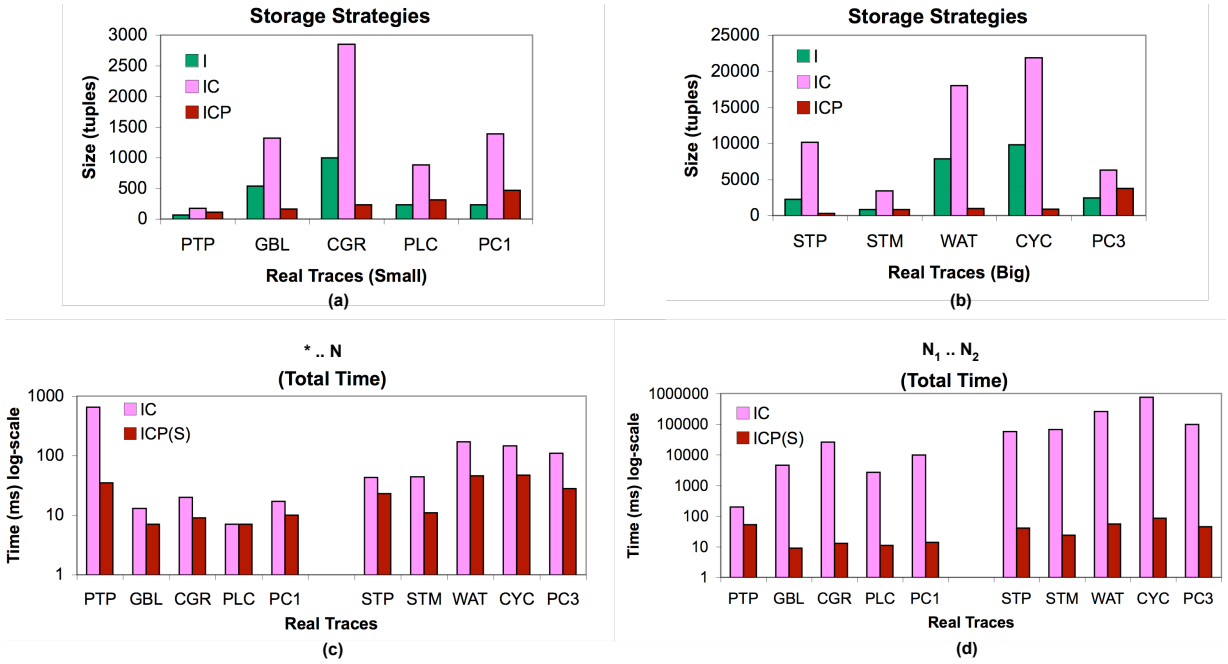


Figure 14: (a) and (b) shows size for storing real traces in various storage strategies. (c) and (d) shows time for evaluating constructs *..N and N_1 ..N_2 over these storage strategies.

compare this result with the results for the synthetic traces, we see that as the number of dependencies increases, *IC* will perform even worse.

Analysis. Our detailed experimental evaluation demonstrates that *ICP* not only requires less storage, but evaluating QLP queries over *ICP* is faster and scales with increasing complexity of traces. In particular, our optimized set-based approach $ICP(S)$ for evaluating QLP path expressions is both efficient and scalable.

6. RELATED WORK

Conventional provenance approaches (e.g., [19, 17, 5]) largely assume workflow models are based on *transformation semantics*, whereas workflow systems that work over structured data (e.g., [7, 26, 23, 27]) often employ *update semantics*, i.e., where only a portion of incoming data is modified by each workflow step. Applying conventional provenance approaches to such models results in provenance information that is either too coarse or potentially incomplete and even incorrect, which can lead to incorrect analysis of scientific results [3]. Our provenance model subsumes conventional approaches for representing workflow provenance by supporting workflow computation models that permit multiple invocations of processes (e.g., for pipelining and loops), structured data, and update semantics. In prior work, we show how existing models (including OPM [19]) can be mapped to our provenance model [3].

Approaches for querying provenance are largely based on physical data representations [13] (e.g., relational, XML, or RDF schemas), where users express provenance queries through corresponding query languages (i.e., SQL, XQuery, or SPARQL). Provenance queries often require computing transitive closures over dependency relations, and expressing such queries using standard approaches is typically done using recursion or stored procedures [16, 11, 2]. Expressing such queries is both cumbersome and error-prone, and requires considerable user expertise. Instead, high-level languages such as QLP provide a separation between the logical provenance model and its underlying physical representation, which allows for the use of different representation schemes and additional optimization techniques. Our approach, in particular, automatically translates QLP queries to equivalent relational queries expressed against the provenance storage schemes described in [2].

Standard approaches for querying provenance information (e.g., [10, 17, 29, 12, 6]) return sets of nodes (either sets of data items or process invocations) as the query result. This approach requires additional steps (queries) to reconstruct causal relations among nodes within a query answer. Instead, QLP is closed under lineage relations, where answers to lineage queries are sets of lineage dependencies (edges) forming provenance subgraphs, and thus query results are "provenance preserving." This approach has a number of advantages, e.g., for supporting provenance views, incremental querying, and for supporting visualization applications [13, 7].

Our approach is similar to a number of approaches for querying graph structures. In [15], a general query langauge based on graph grammars is presented in which queries return subgraphs. However, whereas our implementation uses a relational database system to store and query provenance graphs, the approach in [15] requires entire graph structures to be stored in main memory, and recursive patterns over graphs (e.g., similar to our '..') are not supported. Similarly, semi-structured query languages (e.g., Lorel [1] and Florid [21]) often include so-called "path variables", which can be used to query over and return paths (i.e., the nodes) between nodes. However, while a part of the query language of these systems, path variables are generally not implemented (e.g., see [1, 21]). Additionally, the approach used in QLP differs from that of path variables in that query results are sets of lineage relations that *implicitly* denote paths between nodes as opposed to directly returning the paths themselves. This in turn offers advantages for query composition and efficient evaluation (as described in Section 4).

Similar to QLP, vtPQL (used in VisTrails [10]) defines provenance-specific query constructs. The primary construct in vtPQL for answering lineage queries related to invocations is

upstream(x), which return all modules (actors) that procede x in the workflow definition. However, vtPQL assumes only a *single* lineage path between two such modules, and thus would return incorrect results in the case where multiple paths exist between nodes.

The QLP construct exists$(n_1 .. n_2)$ corresponds to a reachability query [18, 28] over lineage graphs. Besides simple paths, our implementation can efficiently answer more complex reachability queries for paths $p = s_1 .. s_2 .. s_3 \cdots s_m$ of length $m > 2$ in which each step s can evaluate to a set of nodes. Thus, our implementation can also efficiently determine whether a lineage graph satisfies relatively complex path expressions.

7. CONCLUSION

We have presented a general approach for querying provenance using a novel query language (QLP) that provides specialized constructs for querying over lineage and structural relations introduced during scientific workflow runs. Answers to lineage queries are sets of lineage dependencies (edges) forming provenance subgraphs, which simplifies the expression of complex queries and allows query results to be easily queried and visualized. This work extends our prior work on efficiently storing [2] and querying [3] scientific workflow provenance by presenting (i) a formal semantics for QLP constructs; (i) a set of novel query optimization techniques that leverage the lineage-graph reduction approaches presented in [2]; and (iii) a detailed experimental evaluation based on our QLP implementation that demonstrates the efficiency and scalability of our approach. We have shown that our implementation can simultaneously reduce the amount of storage required to represent scientific workflow provenance without negatively affecting query performance. We have also shown that unlike using standard approaches (often based on in-memory implementations, e.g., [29, 15, 21]), answering QLP queries using our optimization techiques over a relational database system is both feasible and scales with the size of provenance information and query complexity. Our optimizations can also be used in more general settings to efficiently answer a broad range of path queries over labeled, acyclic digraphs.

Acknowledgments. This work supported in part by NSF grants IIS-0630033, OCI-0722079, IIS-0612326, and DOE grant DE-FC02-07ER25811.

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