Distributed Relational Algebra at Scale

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ABSTRACT

Relational algebra forms a basis of primitive operations useful for applications in graphs, networks, program analysis, deductive databases, and logic. Despite its expressive power, relational algebra has not received the same attention in high-performance computing research as linear algebra, stencil computation, map-reduce or graph analytics. In this paper we present a set of efficient algorithms to effectively parallelize key relational algebra primitives. We introduce an hash-tree approach to Finally we demonstrate the scalibility of our implementation through the fixed point algorithm that computes the transitive closure of a large graph at scale.

CCS CONCEPTS

• **Computer systems organization** → **Embedded systems**; *Redundancy*; Robotics; • **Networks** → Network reliability.

KEYWORDS

datasets, neural networks, gaze detection, text tagging

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1 INTRODUCTION

Implementing application-specific code on supercomputers requires addressing the fundamental underlying primitives of an algorithm in a way that is flexible and scalable. Significant progress has been made on a wide variety of important problems due to a rigorous exploration of common high-performance primitives such as stencil computations, floating-point arithmetic, numerical integration, and sparse linear algebra.

Relational algebra is crucial primitive for a wide range of analytic problems in graphs, machine learning, logic programming, program analysis, deductive databases, and formal verification, that has been the subject of great interest in the literature, but has had limited exploration on supercomputers, and at scale. Two central problems to scaling operations on relations, such as union, selection, projection, and join, have been (a) how to represent distributed relations in a way that is amenable to efficient parallel operations, and (b) how to handle communication to coordinate distinct portions of the distributed workload.

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While some recent progress has been made in addressing these issues, (a) in particular, no approach has yet provided a general framework that makes applications using a pipeline of *repeated* operations on relations—for fixed-point interation, supporting applications such as Datalog and program analysis—possible at scale. For such applications to be implemented on distributed, many-core systems, existing algorithms that distribute relations among available cores, perform a single operation, and return in map-reduce fashion are not suitable as repeated operations require efficient granular communication at each step.

In this paper, we present a hybrid approach to representing relations on networked machines and performing efficient distributed operations on them, building on the current state of the art for single-node parallelism. Interestingly, in addressing the communication issue, we find that MPI's all-to-all communication paradigm suits relational algebra best. Today's supercomputers have very high speed interconnects—data can be transmitted between processes with very low latency. When used under the right configuration, all-to-all communication which is known to be the most intensive mode of communication can scale well.

Contributions. In particular, we make the following specific contributions to the literature:

(1) We present novel hybrid hash-tree based algorithms for distributed relational algebra.
(2) We present a scalable implemetation and experiments for a fixed-point algorithm employing distributed relational algebra: computing the transitive closure of a graph.
(3) We demonstrate scalability of transitive closure up to 65,536 processes, producing a graph with more than 260 billion edges. To the best of our knowledge, this is the largest transitive closure discussed in the literature.

We understand our implementation to be the first truly scalable distributed relational algebra that addresses inter-process communication, permitting fixed-point interation, and laying the foundation for solving massive logical inference problems, graph problems, and more on supercomputers.

2 RELATIONAL ALGEBRA

Relational algebra (RA) provides a basis of operations on relations (i.e., predicates, or sets of tuples) sufficient to implement a broad range of algorithms for databases and queries, data analysis, machine learning, graph problems, and constraint logic problems []. Scaling these underlying primitives, and finding an effective strategy for parallel communication to distribute them across multiple nodes, is thus a avenue for scaling and distributing algorithms for high-performance program analyses, deductive databases, among other applications. This section reviews the standard relational operations union, product, intersection, natural join, selection, renaming, and projection, along with their use in implementing two closely related example applications: graph problems and bottom-up datalog solvers.

The Cartesian product of two finite enumerations D_0 and D_1 is defined $D_0 \times D_1 = \{(d_0, d_1) \mid \forall d_0 \in D_0, d_1 \in D_1\}$. A *relation* $R \subseteq D_0 \times D_1$ is some subset of this product that defines a set of associated pairs of elements drawn from the two domains. For example, if R were the relation ($\geq$) over natural numbers, both domains D_0 and D_1 would be $\mathbb{N}$ and the relation could be defined $(\geq) = \{(n_0, n_1) \mid n_0, n_1 \in \mathbb{N} \wedge n_0 \geq n_1\}$. Any relation R can also be viewed as a predicate P_R where $P_R(d_0, \ldots, d_k) \iff (d_0, \ldots, d_k) \in R$, or as a set of tuples, or as a database table.

We make some standard assumptions about relational algebra that differ from those of traditional set operations. Specifically, we assume that all our relations are sets of flat (first-order) tuples of natural numbers with a fixed, homogeneous arity. This means that the relation $(\mathbb{N} \times \mathbb{N}) \times \mathbb{N}$ contains the tuple $(1, 2, 3)$, and not $((1, 2), 3)$. It also means that although our approach extends naturally to relations over arbitrary enumerable domains (such as integers, booleans, symbols/strings, lists of integers, etc)—we make the assumption that natural numbers may be used in the place of other enumerable domains when they are needed. Finally, this means that for operations like union or intersection, both relations must by union-compatable by having the same arity and column names.

... talk about names as indices?

2.1 Standard RA operations

...

Cartesian product. The product of two relations R and S is defined: $R \times S = \{(r_0, \ldots, r_k, s_0, \ldots, s_j) \mid (r_0, \ldots, r_k) \in R \wedge (s_0, \ldots, s_j) \in S\}$.

Union. The union of two relations R and R' may only be performed if both relations have the same arity but is otherwise set union: $R \cup R' = \{(r_0, \ldots, r_k) \mid (r_0, \ldots, r_k) \in R \vee (r_0, \ldots, r_k) \in R'\}$.

Intersection. The intersection of two relations R and R' may only be performed if both have k arity but is otherwise set intersection: $R \cap R' = \{(r_0, \ldots, r_k) \mid (r_0, \ldots, r_k) \in R \wedge (r_0, \ldots, r_k) \in R'\}$.

Projection. Projection is a unary operation that removes a column or columns from a relation—and thus any duplicate tuples that result from removing these columns. Projection of a relation R restricts R to a particular set of dimensions $\alpha_0, \ldots, \alpha_j$, where $\alpha_0 < \ldots < \alpha_j$, and is written $\Pi_{\alpha_0, \ldots, \alpha_j}(R)$. For each tuple, projection retains only stated columns: $\Pi_{\alpha_0, \ldots, \alpha_j}(R) = \{(r_{\alpha_0}, \ldots, r_{\alpha_j}) \mid (r_0, \ldots, r_k) \in R\}$.

Renaming. Renaming is a unary operation that renames (i.e., reorders) columns. Renaming columns can be defined in several different ways, including renaming all columns at once. We define our renaming operator, $\rho_{\alpha_i/\alpha_j}(R)$, to swap two columns, α_i and α_j where $\alpha_i < \alpha_j$—an operation that can be repeated to rename/reorder as many columns as desired:
$\rho_{\alpha_i/\alpha_j}(R) = \{(\ldots, r_{\alpha_j}, \ldots, r_{\alpha_i}, \ldots) \mid (\ldots, r_{\alpha_i}, \ldots, r_{\alpha_j}, \ldots) \in R\}$.

Selection. Selection is a unary operation that restricts a relation to tuples where a particular column matches a particular value. As with renaming, a selection operator may alternatively be defined to allow multiple columns to be matched at once, or to allow inequality or other predicates to be used in matching tuples. In our formulation, selection on multiple columns can be accomplished by repeated selection on a single column at a time. Selecting just those tuples from relation R where column α_i matches a value v is defined:
$\sigma_{\alpha_i = v}(R) = \{(r_{\alpha_0}, \ldots, r_{\alpha_k}) \in R \mid r_{\alpha_i} = v\}$.

Selecting just those tuples from relation R where the values in columns α_i and α_j must match is defined:
$\sigma_{\alpha_i = \alpha_j}(R) = \{(r_{\alpha_0}, \ldots, r_{\alpha_k}) \in R \mid r_{\alpha_i} = r_{\alpha_j}\}$.

Natural Join. Two relations can also be *joined* into one on a subset of columns they have in common. Join is a particularly important operation that combines two relations into one, where a subset of columns are required to have matching values, and generalizes both intersection and Cartesian product operations.

Consider an example of two tables in a database, one that encodes a system's users' `emails` (including their username, email address, and whether it's verified) and another that encodes successful `logins` (including a username, timestamp, and ip address):

emails

username	email	verified
samp	samwow@gmail.com	1
samp	samp9@uab.edu	0
karenk	karenk5@uab.edu	1

logins

username	timestamp	ipaddr
samp	1554291414	162.103.150.12
karenk	1554181337	171.31.15.120
karenk	1554219962	155.28.11.102
karenk	1554133720	171.31.15.120

A join operation on these two relations, written `users` $\bowtie$ `logins`, yields a single relation with all five columns: username, email, passhash, timestamp, address. For columns the two relations have in common, the natural join only considers pairs of tuples from the two input relations where the values for those columns match, as in an intersection operation; for other columns, the natural join computes all possible combinations of their values as in Cartesian product. If both input relations share all columns in common, a join is simply intersection and if both input relations share no columns in common, a join is simply Cartesian product. For the above tables, the natural join is shown:

emails $\bowtie$ logins

username	email	verified	timestamp	ipaddr
samp	samwow@...	1	...414	162...
samp	samp9@...	0	...414	162...
karenk	karenk5@...	1	...337	171...
karenk	karenk5@...	1	...962	155...
karenk	karenk5@...	1	...720	171...

For example, if we wanted to compute all email addresses and ip addresses that may be associated, we could compute the join of these two relations and then project the join down to these two attributes alone. Note that one row is removed because it becomes a duplicate after projection:

$$\Pi_{\texttt{email}, \texttt{ipaddr}}(\textbf{emails} \bowtie \textbf{logins})$$

email	ipaddr
samwow@gmail.com	162.103.150.12
samp9@uab.edu	162.103.150.12
karenk5@uab.edu	171.31.15.120
karenk5@uab.edu	155.28.11.102

In this example, we've shown relations with associated attribute (column) names (e.g., `email`, `ipaddr`). In our formalization of relations, we treat columns as ordered and identified by their index instead—naturally a programming model, RDBMS, or API for relations will likely associate these indices with their symbolic names. As formalized, the `emails` relation would be a set of tuples:

$$R_{\texttt{emails}} = \{\ (0, 0, 1),\ (0, 1, 0),\ (1, 2, 1)\ \},$$

Where the attributes `username`, `email`, and `verified` are stored in columns 0, 1, and 2, respectively, the string "`samp`" is interned as username 0, the string "`karenk`" is interned as username 1, and the three emails are interned as emails 0, 1, and 2.

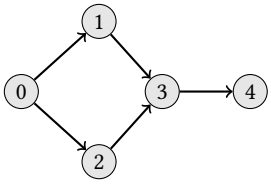
To formalize natural join as a operation on such a relation, we parameterize it by the number of indices that must match, assumed to be the first j of each relation (if they are not, a renaming operation must come first). The join of relations R and S on the first j columns is written $R \bowtie_j S$ and defined:

$$R \bowtie_j S = \{\ (r_0, \ldots, r_k, s_j, \ldots, s_m) \mid (\ldots, r_k) \in R \wedge (\ldots, s_m) \in S \wedge \bigwedge_{i=0..j-1} r_i = s_i\ \}$$

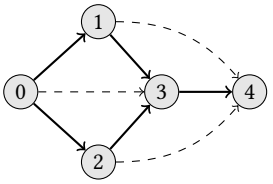
2.2 Application: transitive closure

One of the simplest common algorithms that may be implemented efficiently as a loop over high-performance relational algebra primitives, is computing the *transitive closure* (TC) of a relation or graph. Consider a relation $G \subseteq \mathbb{N}^2$ encoding a graph where each point $(a, b) \in G$ encodes the existence of an edge from node a to node b.

For example, consider graph G (shown below) where $G = \{(0, 1), (1, 3), (0, 2), (2, 3), (3, 4)\}$.



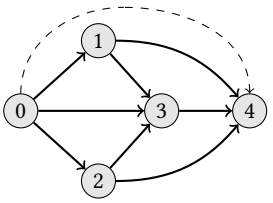
Renaming to swap the columns of G, results in a graph $\rho_{0/1}(G)$ where all arrows are reversed in direction. If this graph is joined with G on only the first column (meaning G is joined on its second columns with G on its first column), we get a set of triples (b, a, c)—specifically $\{(1, 0, 3), (2, 0, 3), (3, 1, 4), (3, 2, 4)\}$—representing paths of length two in the original graph where a leads to b which leads to c. Projecting out the first column yields pairs (a, c) encoding paths of length two from a to c in the original graph G. If this is unioned with the original G, we obtain a relation encoding paths of length one or two in G. This graph, $G \cup \Pi_{\alpha_1, \alpha_2}(\rho_{0/1}(G) \bowtie_1 G)$, is shown below with new edges (paths of length two) shown in dashes.



We can encapsulate this step in a function F_G which takes as input a relation T encoding a graph and returns the graph G unioned with T's edges extended with G's edges.

$$F_G(T) \triangleq G \cup \Pi_{\alpha_1, \alpha_2}(\rho_{0/1}(G) \bowtie_1 T)$$

The graph shown above can be produced by $F_G(G)$ and the graph G is returned if the input graph T is empty: $F_G(\varnothing)$, or $F_G(\bot)$. If F_G is repeatedly applied, the results encodes ever longer paths through G. In this case for example, the graph $F_G(F_G(G))$ or ${F_G}^3(\bot)$ encodes the transitive closure of G—all paths in G reified as edges.



In the general case, for any graph G, there exists some $n \in \mathbb{N}$ such that ${F_G}^n(\bot)$ encodes the transitive closure of G. The transitive closure may be computed by repeatedly applying F_G in a loop until reaching an n where ${F_G}^n(\bot) = {F_G}^{n-1}(\bot)$ in a process called *fixed-point iteration*. In the first iteration, paths of length 1 are computed; in the second, paths of length 1 or two are computed, and so forth. After the longest path in G is found, just one additional iteration is necessary as a fixed-point check to confirm that the final graph has stabilized.

2.3 Application: Datalog

Computing transitive closure is a simple example of logical deduction. From paths of length 0 (an empty graph) and the existence of edges in graph G, we may deduce the existance of paths of length $0 \ldots 1$. From paths of length $0 \ldots n$ and the original edges in graph G, we may deduce the existance of paths $0 \ldots n + 1$ edges long. The function F_G above performs a single round of this inference, finding paths one edge longer than any found previously and exposing new deductions for the next iteration of F_G to make. When the computation reaches its fixed point, a solution has been found because no further paths may be deduced from the available facts.

In fact, the function F_G is just an encoding in relational algebra of the transitivity propery itself, $T(a, b) \wedge T(b, c) \implies T(a, c)$, a logical constraint for which we desire a minimal solution. A graph T satisfies this property exactly when T is a fixed-point for F_T.

Solving logical problems in this way is precisely the strategy of *bottom-up logic programming*. Bottom-up logic programming begins with a set of facts (such as $T(a, b)$—the existence of an edge in a graph T) and a set of inference rules (such as $T(a, b) \wedge T(b, c) \implies T(a, c)$) and performs a fixed-point calculation, accumulating new facts that are immediately derivable, until reaching a minimal set of facts consistant with all rules.

Datalog is a bottom-up logic programming language supporting a restricted logic corresponding to first-order HornSAT—the satisfiability problem for conjunctions of Horn clauses. A *Horn clause* is a disjunction of atoms where all but one is negated: $a_0 \vee \neg a_1 \vee \ldots \vee \neg a_j$. By DeMorgan's laws we may rewrite this as $a_0 \vee \neg(a_1 \wedge \ldots \wedge a_j)$ and note that this is an implication: $a_0 \leftarrow a_1 \wedge \ldots \wedge a_j$. In first-order logic, atoms are predicates with universally quantified variables.

A Datalog program is a set of rules $P(x_0, \ldots, x_k) \leftarrow Q(y_0, \ldots, y_j) \wedge \ldots \wedge S(z_0, \ldots, z_m)$ and its input is a database of facts called the *extensional database* (EDB). Running the datalog program reifies the *intensional database* (IDB) which extends facts from the EDB with all facts transitively derivable via the program's rules.

In the typical notation of datalog, computing transitive closure of a graph is accomplished with just two rules:

```
path(x,y) :- edge(x,y).
path(x,z) :- path(x,y), edge(y,z).
```

The first says that any edge implies a path (taking the role of the left operand of union in F_G), and the second says that any path (x, y) and edge (y, z) imply a path (x, z) (adding edges for the right operand of union in F_G).

Each Datalog rule may be encoded as a function F (between databases) where a fixed point for the function is guaranteed to be a database that satisfies the particular rule. Atoms in the body (premise) of the implication, where two columns are required to match, are refined using a selection operation; e.g., atom $S(a, b, b)$ is computed by RA $\sigma_{\alpha_1=\alpha_2}(S)$. Conjunction of atoms in the body of the implication is computed with a join operation: e.g., in the second rule above, this is the second column of `path` joined with the first of `edge`, or $\rho_{0/1}(\texttt{path}) \bowtie_1 \texttt{edge}$. These steps are followed by projection to only the columns needed in the head of the rule and any necessary column reordering. Finally, the resulting relation is unioned with the existing relation in the head of the implication to produce F's output, an updated database (e.g., with an updated `path` relation in the examples above).

Once a set of functions $F_0 \ldots F_m$, one for each rule, are constructed, Datalog evaluation operates by iterating the IDB to a mutual fixed point for $F_0 \ldots F_m$.

2.4 Implementation approaches

In our previous discussion of both transitive closure and Datalog, we have elided important optimizations and implementation details in favor of focusing on the main ideas of both. In practice, however, it is inefficient to perform multiple granular RA operations separately to perform a selection, reorder columns, join relations, project out unneeded columns, reorder columns again, etc, when iteration overhead can be eliminated and cache coherence improved by performing loop fusion. In practice, high-performance Datalog solvers perform all necessary steps at once, supporting a generalization of the operations we've discussed that can join, select, reorder variables, project, and union, all at once.

In addition, both transitive closure and Datalog, as discussed above, are using naïve fixed-point iteration, recomputing all previously discovered edges (resp. facts) at every iteration. Efficient implementations are *incrementalized*, only considering facts that can be extended to produce previously undiscovered facts. For example, when computing transitive closure, another relation T_Δ is used which only stores the longest paths—those discovered in the previous iteration. When computing paths of length n, in fixed-point iteration n, only new paths discovered in the previous iteration, paths of length $n-1$, need to be considered as shorter paths extended with edges from G yield paths which must have been discovered already. In the more general cases of Datalog and database theory, this optimization is known as *semi-naïve* evaluation.

Now, we review the two main approaches to encoding relations in a manner amenable to fast RA algorithms. Unsurprisingly, algorithms for computing join, union, selection, etc, depend greatly on the representation used for relations themselves.

Decision diagrams. One approach is the use of decision trees to encode relations. *Decision diagrams* (DDs) such as *binary decision diagrams* (BDDs) and its variants, zero-supressed binary decision diagrams (ZDDs) and algebraic decision diagrams (ADDs), are potentially compact representations of relations, predicates, sets of strings, or sets of sets. In a BDD, each variable (column) storing an integer is decomposed into one variable per bit: a relation R(a,b,c) where each column stores a 64bit integer is encoded as a set of binary strings, each 192 bits long. A BDD encodes the decision procedure of determining inclusion of a string (i.e., tuple, fact) in the set as a tree where each node has two subtrees, one for encoding string suffixes that follow a 0, and one for encoding string suffixes that follow a 1. The root node for a BDD encoding relation $R(a, b, c)$ has two subtrees, one for encoding a set of 191-bit strings with a 0 as the initial bit, and one for likewise encoding suffixes with a 1 as the leading bit. The children of leaf nodes are one of two special ($\bot$ and $\top$) nodes that indicate no strings exist with the encoded prefix or that all strings with the encoded prefix are present in the set.

Algorithms for performing RA on decision diagrams recursively merge nodes of the tree according to the operation being performed, taking time proportional to the size of the structures, and can be highly efficient when the tree is compact. Performant DD libraries like CUDD (CU decision diagram library) perform recursive interning under the hood to improve space efficiency []. In practice, decision diagrams can be highly compact or can blow up exponentially, depending largely on variable ordering (i.e., what determines which bits are near the root). A major practical downside of DDs has been the difficulty of automatically determining a efficient variable ordering given that a representation of domain-specific problems in decision diagrams (via an encoding in Datalog) has already thoroughly obfuscated the meaning behind each bit. Much work has gone into simply trying to learn, or dynamically adapt, a DD's variable ordering to the problem at hand.

Key-value stores. Another approach to encoding relations that has recently shown far greater scalability [], although it is both older and apparently less sophisticated, is to use a hash table, B-tree, prefix tree (trie), or other key-value store to maintain a set of tuples, with support for efficient iterators to directly loop over all facts in a relation when performing RA.

In this approach, a join becomes nested iteration over two or more relations to build up a set of output tuples that can be inserted into a new relation encoded as a key-value store. Unioning can be done by simply inserting tuples into an existing relation. Renaming, projection, and selection, can all be done trivially, on-the-fly, while performing a join, as these are as simple as reordering the variables

of each tuple before an insertion, omitting values from a tuple before insertion, or omitting tuples that do not qualify before insertion.

In a join operation, it is inefficient to iterate over all tuples of two relations if any variables are unified (if the join is not equivalent to Cartesian product). Instead, only the first relation is iterated over in its entirety and an efficient selecting iterator is used to iterate over only those tuples in the second relation where unified variables match. This is accomplished by using a key-value store for tuple keys that is implemented using nested key-value stores for integer keys. Here again variable ordering becomes crucial as columns being selected on must come first. Unlike for DDs however, the variable ordering issue can be solved precisely and statically (at compile time) as the structure of RA operations being performed implies the necessary indices.

Consider the second Datalog rule implementing transitive closure, discussed previously, defining paths in terms of paths and edges. Each iteration of our function F for this rule can be implemented as the following pseudocode:

```
new_delta_path = {}
for [x,y] in delta_path.select_all():
   for [y,z] in edge.select("y", y):
      if path.insert([x,z]) == true:
         new_delta_path.insert([x,z])
delta_path = new_delta_path
```

3 HASH-TREE RELATIONAL ALGEBRA

This section discusses our implementation of distributed relational algebra. We employ a hybrid approach we call *hash-tree* relational algebra that consists of nesting B-tree key-value stores within a hash-table that can be partitioned across multiple cores or MPI nodes. As discussed in the previous section, the key-value store approach to encoding relations requires nested maps to support efficient join (and select) operations. In a typical join, it will be necessary to iterate over all tuples in a relation where particular columns match a value or values taken from the first operand of join—in which case the variable being matched should come first and be a key in the outermost B-tree. The relation is thus explicitly indexed on this column.

In our implementation, a relation $R(a, b)$ indexed on a is encapsulated in a type `Relation<Relation<void>>` which provides an interface to a B-tree mapping `uint64_t` keys, storing each a, to subrelations over just those values b that are paired with a particular a. In our approach, this nesting of B-trees is extended at the top-level by a hash table so that each value a is also hashed to one of *nproc* (the number of MPI processes being used to host the relation) *buckets*.

Hybrid join. The standard way to parallelize the key-value store approach to relational algebra on multi-core systems is to partition the iteration space of the outermost loop. For example, the Soufflè Datalog solver uses OpenMP to parallelize its join operations, first partitioning the outermost key-value store into multiple disjoint iterators—one for each available thread. Soufflè's join algorithm is nearly identical to our previous pseudocode for join, except that it adds an outer parallel for loop.

```
new_delta_path = {}
pfor part_iter in delta_path.partition():
   for [x,y] in part_iter:
      for [y,z] in edge.select("y", y):
         if path.insert([x,z]) == true:
            new_delta_path.insert([x,z])
delta_path = new_delta_path
```

3.1 Distributed hash-tree join

Our hybrid hash-tree structure for relations makes this partitioning explicit as physically separate relations stored in distinct hash-table buckets—each owned by a dedicated MPI process. Join operations then decompose into a separate join for each bucket, followed by hashing of output tuples, and a communication phase to insert these tuples into the output relation. In experiments designing our join operation, we found that, as hashing distributes key values evenly across buckets, MPI's all-to-all communication paradigm was actually most efficient for inserting output tuples in their receiving buckets (i.e., on processes hosting in the output relation).

In Figure 1 we show the process for computing a single iteration of a distributed transitive closure computation. T (i.e., T_Δ as we implement an incrementalized TC algorithm) is joined with G on a per-bucket basis (the diagram shows three color-coded buckets). Tuples in $T(x, y)$ are indexed on the second column (y) and tuples in $G(y, z)$ are indexed on the first column (y). This makes it possible to perform local (intra-bucket) joins as each tuple $(x, y) \in T$ is guaranteed to have all matching tuples $(y, z) \in G$ stored in the same bucket, managed by the same MPI process. Each resulting triple (x, y, z) has its middle column projected out on-the-fly as it is produced, and, as the resulting tuple (x, z) must be inserted into T, a relation indexed on its second column, each new edge is hashed and assigned to bucket $hash(z)\%nprocs$ in the output relation (T). As this bucket will likely not be managed by the local MPI process, a communication phase is required to actually perform insertion of each output tuple in its output relation. As each output tuple is produced it is staged in one of *nprocs* packets, ready to be sent across the network to the MPI process managing its bucket. Finally, an all-to-all communication phase is used to reorganize the output of the join operation—preparing T for subsequent fixed-point iterations. As tuples are received by their host process, they are inserted into the local B-tree structure, eliminating duplicates.

3.2 Distributed hash-tree union

We present two algorithms for distributed unions, naïve hash-tree union and buffered hash-tree union. As the name suggests buffered hash-tree union buffers data across all relations that need to be unioned before performing any communication or insertions and performs the union concurrently in a single step. While performing a union of n relations, naïve hash-tree union involves n epochs of communication and computation—one for each relation—as opposed to buffered hash-tree union that uses buffering to limit the number of communication and computation epochs to one.

Naïve hash-tree union is concurrent in processing each relation being unioned, but unions each relation in a separate step. Naturally, our buffered implementation has an extra memory overhead as opposed to the naïve implementation where all graphs that need to be unioned are processed one at a time, however it is

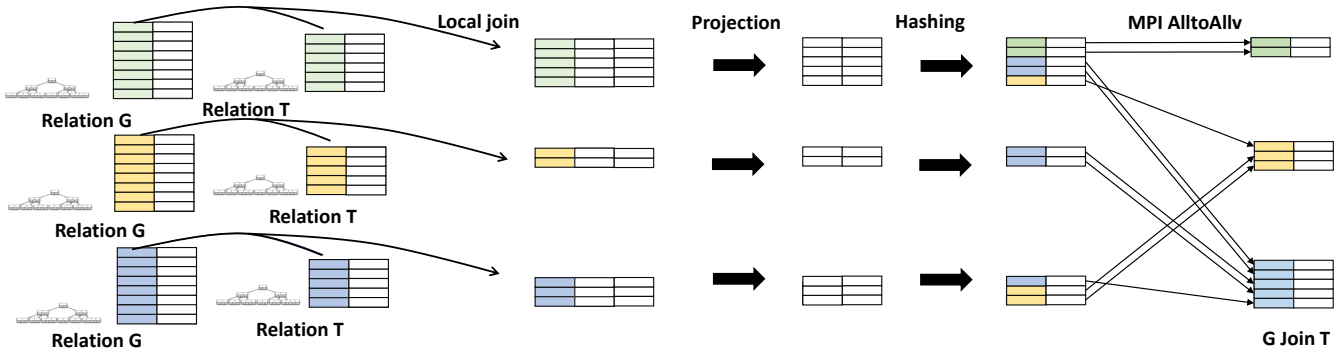


Figure 1: Schematic Diagram to show different phases of hash-tree join.

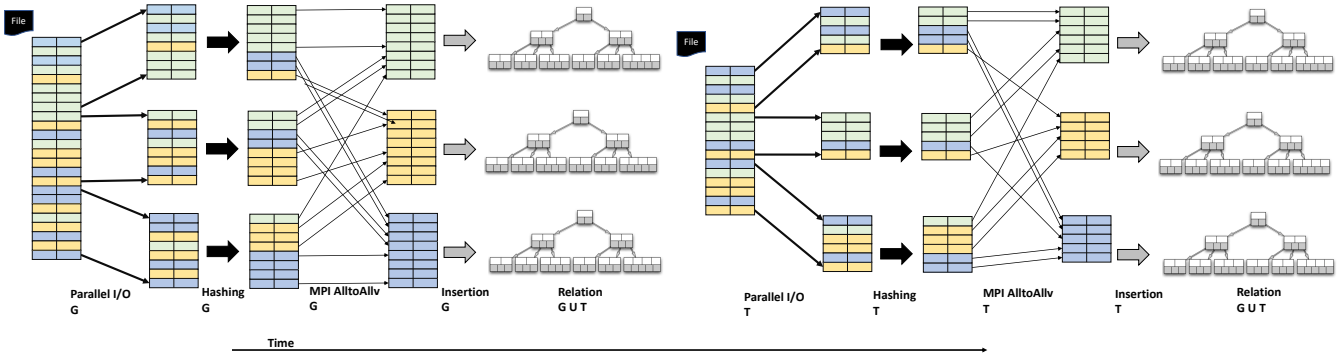


Figure 2: Schematic Diagram to show different phases of naive hash-tree union.

more representative of real applications (such as Datalog, program analysis, etc) where each relation being unioned would have a set of nodes hosting it and tuples across multiple relations could all be transmitted and inserted into a new relation concurrently.

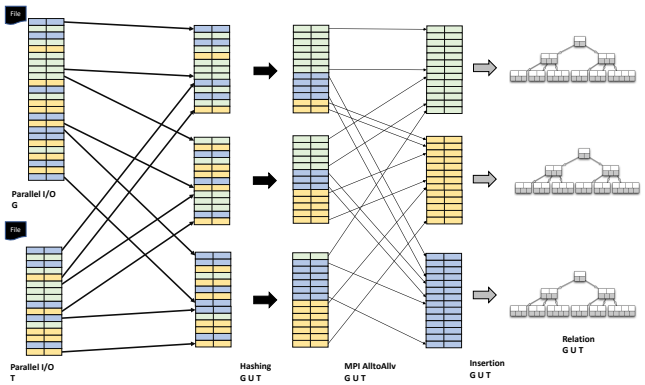


Figure 3: Schematic Diagram to show different phases of buffered hash-tree union.

The input graphs can be read from files stored on the disk or can be read directly from memory. If the graphs are read from disk, the first phase is that of parallel I/O: processes access disjoint regions of the file to read an equal number of tuples in parallel. Once the tuples are read into memory, each process scans through its tuples and hashes them, grouping tuples into *nprocs* packets, ready to be sent across the network. The target process (i.e., outer hash-bucket) of a tuple is computed based on the hash value of its key. For instance, the target rank of a two column tuple (a, b), where a is the outer key and b the inner key, would be $hash(a)\%nprocs$. We also perform preliminary deduplication, as these tuples are staged, before transmitting these batches of tuples to minimize communication overhead. The grouping step is followed by an all-to-all communication phase where tuples are sent to the appropriate processes (outer hash buckets). Once tuples arrive at a process, they are inserted into the local relation container. This step performs the important task of deduplication of tuples across relations.

4 EVALUATION

The goal of this section is to evaluate the performance of our distributed hash-tree implementations of join, union and transitive closure at scale. We start by individually studying the computation and communication components of the RA operations. Computation is dominated by insertion of tuples and the major challenge faced is that of deduplication. We therefore study the efficacy of our B-tree-based relation container in isolation. As all our RA operations involve an all-to-all communication phase, we perform a detailed benchmark of MPI's all-to-all communication capability in

Input graph edge count	Union	Join	Transitive Closure	Graph name
412148	✓			
2100225	✓			
6291408	✓			
59062957	✓			
136024430	✓	✓		
180292586	✓	✓		
240023949	✓			

Table 1: List of seven graphs used in our evaluation.

isolation as well. Finally, we benchmark the scaling properties of our distributed parallel union, join, and transitive closure operations over a range of large graphs.

4.1 Dataset and HPC platforms

We performed our experiments using the SuiteSparse Matrix Collection available at [?]. The SuiteSparse Matrix Collection (formerly known as the University of Florida Sparse Matrix Collection), is a large and actively maintained set of sparse matrices that arise in real applications. The Collection is widely used by the numerical linear algebra community for the development and performance evaluation of sparse matrix algorithms. For our experiments, we chose seven graphs (listed in Table **??**) representing a wide range in terms of the number of edges. The transitive closure of a graph with n edges can contain up to n^2 edges (a fully connected graph). The number of edges in the transitive closure of a graph depends on the connectedness and topology of the input graph. For example, the transitive closure of our third graph with 2,100,225 edges contains 276,491,930,625 edges, amounting to 4.4 terabytes of data.

The experiments presented in this work were performed on the Theta Supercomputer at the Argonne Leadership Computing Facility (ALCF). Theta is a Cray machine with a peak performance of 11.69 petaflops, 281,088 compute cores, 843.264 TiB of DDR4 RAM, 70.272 TiB of MCDRAM and 10 PiB of online disk storage. The supercomputer has Dragonfly network topology and a Lustre filesystem.

4.2 Relation container

In this section we evaluate the efficacy and scaling of our per-bucket relation container. We measure performance for two cases: insertions of unique tuples and insertions of tuples with duplicates. In the later set of experiments, each tuple had four duplicates. For both sets of experiments, we compare two implementations of the relation class, one with our B-tree back-end and the other with a hash table back-end. For the hash table experiments, we used `unordered_map` from C++'s standard template library. The results can be seen in Figure 4. The x-axis corresponds to the total number of tuples being inserted and the y-axis is the time taken for this task to finish. We observe that our B-tree-based relation container outperforms the hash-table-based implementation for insertion of all tuple counts. Furthermore, the hash-table-based relation container fails to scale with the insertion of a very large number of tuples. For example, the hash-based relation takes X seconds to insert Y tuples as opposed to only Z seconds taken by the B-tree-based relation. Similar results can be observed for insertion of tuples with duplicates. The B-tree-based relation container successfully deduplicates tuples while maintaining high performance.

4.3 MPI_All_to_Allv

All-to-all communication is central to all of our distributed RA algorithms (Section 3). We use MPI's MPI_Alltoallv function to facilitate all-to-all data communication. MPI_Alltoallv transmits data between all pairs of processes where each process can send a variable amount of data by providing offsets for the input and output data. In this section we study both weak and strong scaling characteristics of MPI_Alltoallv. For both sets of experiments, we varied the number of processes from 2,048 to 32,768. We performed 9 sets of weak scaling experiments. For these 9 experiments, the amount of data transmitted by each process ($data_{process}$) was varied from 4 megabytes (in the 1^{st} set) to 1,024 megabytes (in the 9^{th} set). For an n-process run, every process transmits $data_{process}/n$ units of data to every other process. For strong scaling experiments, we performed 6 sets of experiments, varying the total amount of data generated across processes ($data_{total}$) from 64 gigabytes (in the 1^{st} set) to 2,048 gigabytes (in the 6^{th} set). The amount of data generated by every process is the same; for example, for an n-process run, and $data_{total}$ units of data, every process produces $data_{total}/n$ units of data. A process then transmits $data_{total}/n^2$ units of data to every other process. The results of both weak and strong scaling experiments can be seen in Figure 5.

For both strong and weak scaling runs, we observe a decline in performance with overall decreasing workload. For instance, with strong scaling, the 6^{th} set of experiments, where total workload is 2,048 gigabytes, shows near perfect scaling when the number of processes is doubled from 2,048 (18.5 seconds) to 4,096 (7.3 seconds) to 8,192 (4.5 seconds). After 8,192 processes, although total time continues to come down with increasing process count, we observe that the rate of improvement drops off. Furthermore, looking at the 6^{th} set of experiments, where total workload is 64 gigabytes, we observe relatively poor scaling characteristics across the entire process range. Both these observations may be attributed to an overall reduction in per-process workload. With less data to transmit, total time is dominated by initialization costs as opposed to actual data-transmission cost. For example, with total workload of 64 gigabytes, at 4,096 processes, every process gets a workload of only 16 megabytes (64 gigabytes /4096), and ends up sending 8 kilobytes (16 megabytes /4096) of data to every other process. Similarly, for weak scaling experiments as well, when the amount of data exchanged is substantial, we see almost perfect scaling. For example, when the amount of data transmitted by every process is 1024 megabytes, we observe almost perfect scaling, whereas when the amount of data sent by every process is small (e.g., 4 megabytes) we observe poor scaling.

In the context of communication requirements for distributed RA operations, we find the scaling trends of MPI_alltoallv to be encouraging. In general, for a given workload (i.e., overall tuple count for RA operations), there will always be a range of processes that exhibits good all-to-all scaling characteristics. What remains is the challenge of identifying the ideal process count to balance the trade-off between computation and communication. As we observe

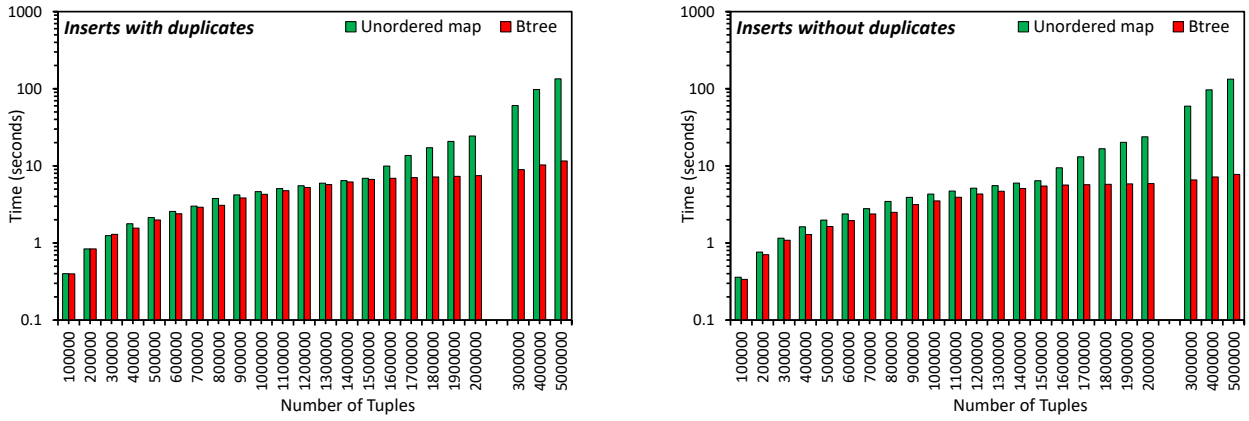


Figure 4: Performance evaluation of our relation class implemented as a B-tree vs unordered map. (left) All tuples are distinct; (right) There are four duplicates of every tuple. Relation implemented as a B-tree out-performs the unordered-map implementation for both cases.

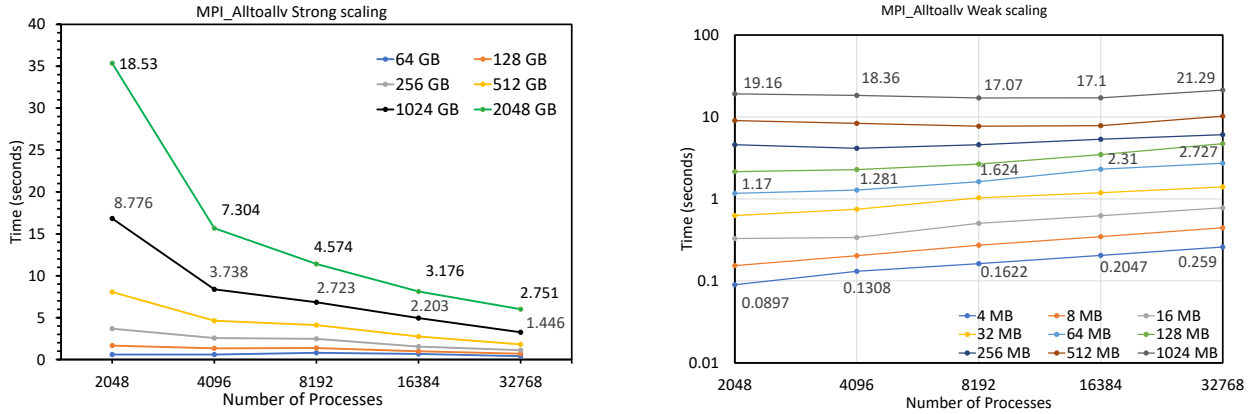


Figure 5: Strong (left) and Weak (right) scaling evaluation of MPI_alltoallv function of MPI.

in section 4.6, below, with larger per-process workload computation cost dominates, as opposed to smaller per-process workload where total cost is dominated by communication.

4.4 Distributed Union

We examine strong scaling to benchmark the performance of our distributed hash-tree union. We measure the time to union all 7 graphs listed in table **??**. The number of processes are varied from 64 to 4,096. The total number of edges across all 7 graphs is 664,659,334 (9.9 gigabytes of data). The union of all 7 graphs has 424,592,810 edges, indicating significant overlap among the graphs.

We benchmark the performance of both buffered hash-tree join and naïve hash-tree join. Performance of both techniques can be seen in Figure 6. We observe two trends: at all process counts, buffered hash-tree union outperforms naïve hash-tree union. This trend can be attributed to an optimized data communication phase associated with buffered unions. Naïve one-by-one union leads to communication involving a small number of large-sized data packets as opposed to the buffered union that involves communication with a large number of small-sized data packets. The other crucial trend is that the union phase only scales to 1024 cores, this can be attributed to an increase in communication time at higher core

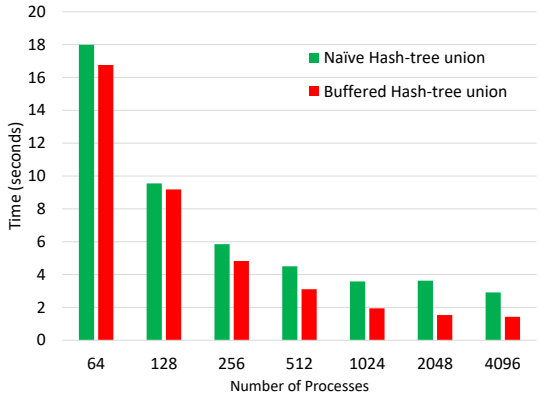


Figure 6: Strong scaling result of hash-tree union.

counts associated with movement of many small-sized data packets. This result corroborates the trend seen in Section **??**. At 2,048 and 4,096 processes, even though the insertion time is reduced, the per-process workload becomes small, impeding scalability of the communication phase.

It can be concluded that for this particular union task (7 graphs) 1024 is the ideal degree of parallelism, as that balances the communication and computation tasks best.

4.5 Distributed Join

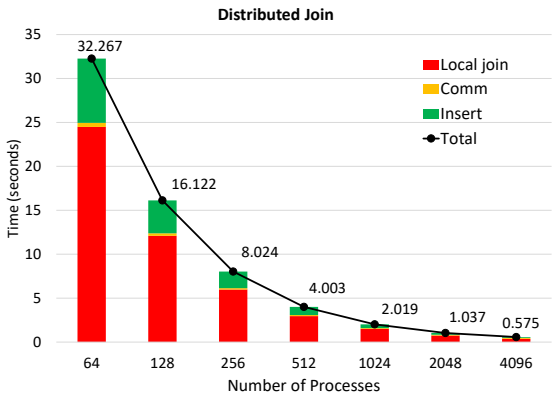


Figure 7: Strong scaling result of hash-tree join.

As with distributed union, we examine strong scaling to benchmark the performance of our distributed join. We perform hash-tree join between two graphs with edge counts 136,024,430 and 180,292,586. The join operation yields a graph with X number of edges. The number of processes are varied from 64 to 4, 096. Once both relations are initialized across all processes (after parallel I/O, hashing, communication and insertions), we initiate the join operation. We plot the scaling results for join in Figure 7. We observe trends similar to distributed union. Join only scales up to X cores, after which communication cost starts to dominate and we observe overall decline in performance.

4.6 Transitive closure

In this section we benchmark a transitive closure computation using our distributed RA and the algorithm discussed in section 3. The transitive closure (T) of an input graph (G) is iteratively extended by adding new paths discovered by a join operation until a fixed point is reached, and no new paths can be added to T. Every iteration is comprised of four phases: 1) a local join 2) all-to-all network communication 3) insertion of new tuples 4) checking if a fixed point was reached.

We performed detailed strong scaling analysis for two graphs, with edge count 412,148 (graph $G1$) and 2,100,225 (graph $G2$). For $G1$ we varied the number of processes from 64 to 8,192, while for $G2$ we varied the number of processes from 4, 096 to 65,536. $G1$ attained its fixed point after 2,933 iterations, generating a total of 1,676,697,415 edges (25 gigabytes). $G2$ attained its fixed point after 2,956 iterations, generating a total of 276,491,930,625 edges ($4terabytes$). The results are plotted in Figure 8. As can be seen in the figure, our approach takes 1000 seconds at 65,536 cores to compute the transitive closure of graph $G2$. To the best of our knowledge, this is the first implementation that has successfully computed the transitive closure of such a large graph.

Further, looking at the graph we obtain for $G1$ we observe considerable scaling up to 1, 024 processes; for 2, 048 and 4, 096 processes, the runs are completely dominated by communication time. This observation again corroborates our strong scaling benchmarking results, where all-to-all communication stops scaling in the presence of many small-sized data packets. For $G1$ we can conclude that 1024 is the ideal scale for computing transitive closure. We observe similar trend with graph $G2$: communication time begins to dominate performance at high core counts of 32,768 and 65,536.

5 RELATED WORK

Hash join is the most popularly used method to parallelize inner join operation. This algorithm involve partitioning the input data so that they can be efficiently distributed to the participating processes. This approach was first introduced in [**?**] in 1988. A lot of work such [**?**] and [**?**] since then has built on top of this approach. Our approach differs from this method as we implement an hybrid approach where we add an extra layer of fast access and lookup data structure at every process. Moreover, ours is the first real demonstration of relational algebra at HPC scale.

More recently [**?**], there has been a concerted effort to implement JOIN operations on clusters using an MPI backend. The commonly used radix-hash join and merge-sort join have been re-designed for this purpose. Both these algorithms involve a hash-based partitioning of data so that they are be efficiently distributed to the participating processes and are designed such that inter-process communication is minimized. In both of these implementations

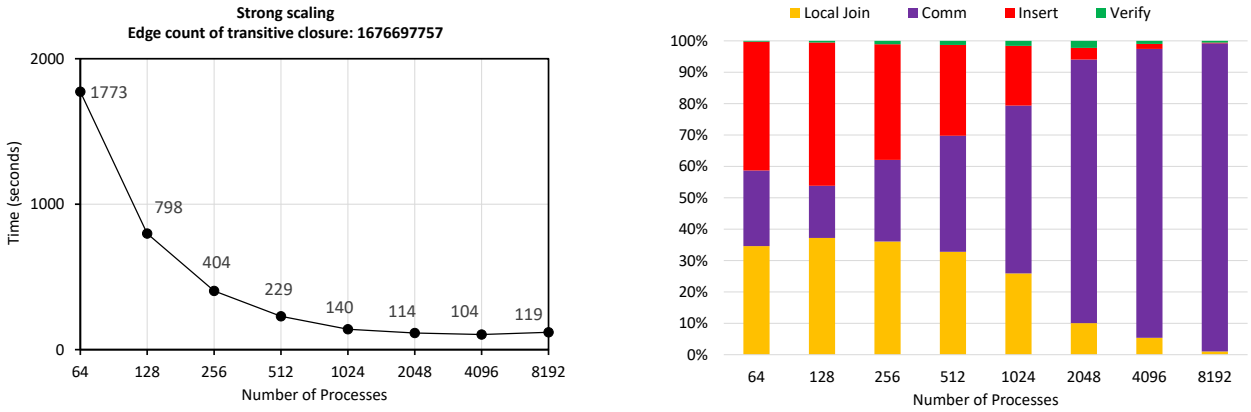


Figure 8: Transitive closure of a graph with X edges.

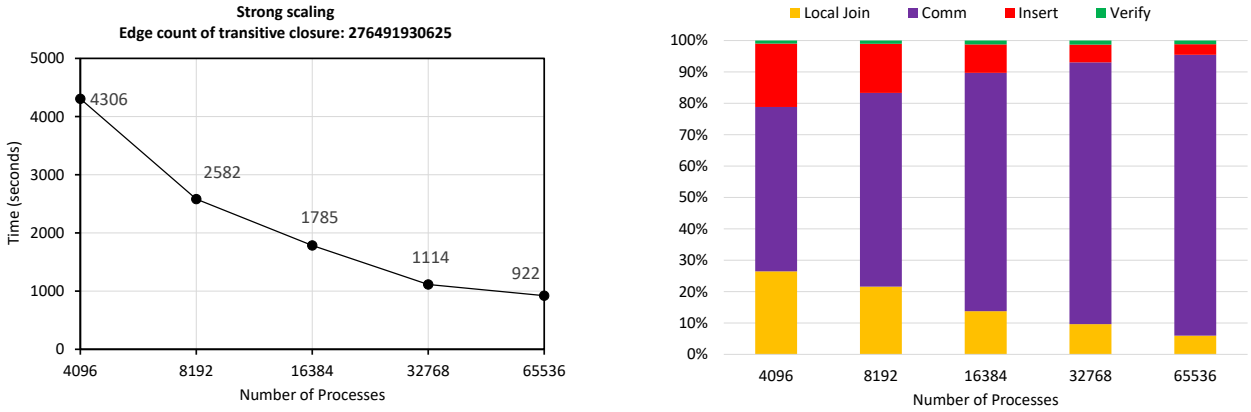


Figure 9: Transitive closure of a graph with X edges.

one-sided communication is used for transferring data between process. This implementation only involved

There has been some work in the past to scale RA operations on GPUs. For example, Redfox is a single-node GPU [**?**] implementation of RA primitives. Other work such as [**?**] and [**?**] have also explored the usage of GPUs to scale dedicated RA task like the triangle listing problem.

Our implementation heavily relies on all to all data communication. We use MPI_alltoallv function to transmit data from all processes to every other process. MPI_Alltoallv is one of the most communication intense collective operation used across parallel applications such as CPMD [**?**], NAMD [**?**], LU factorization, Fast Fourier Transform and matrix transpose. A lot of research [**?**], [**?**], [**?**] has gone into developing scalable implementations of collective operations; most of the existing HPC platforms therefore have scalable implementation of all to all operations.

6 CONCLUSION

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