Parallelizing Sequential Graph Computations

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This paper presents GRAPE, a parallel GRAPh Engine for graph computations. GRAPE differs from prior systems in its ability to parallelize existing sequential graph algorithms as a whole, without the need for recasting the entire algorithms into a new model. Underlying GRAPE are a simple programming model, and a principled approach based on fixpoint computation that starts with partial evaluation and uses an incremental function as the intermediate consequence operator. We show that users can devise existing sequential graph algorithms with minor additions, and GRAPE parallelizes the computation. Under a monotonic condition, the GRAPE parallelization guarantees to converge at correct answers as long as the sequential algorithms are correct. Moreover, we show that algorithms in MapReduce, BSP and PRAM can be optimally simulated on GRAPE. In addition to the ease of programming, we experimentally verify that GRAPE achieves comparable performance to the state-of-the-art graph systems, using real-life and synthetic graphs.

CCS Concepts: • Information systems → Database management system engines: Parallel and distributed DBMSs;

Additional Key Words and Phrases: Graph computations; parallel graph query engines; parallelizing sequential algorithms; convergence; simulation

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1 INTRODUCTION

Several parallel systems have been developed for graph computations, e.g., Pregel [50], GraphLab [49], Giraph++ [63] and Blogel [71]. These systems, however, require users to recast graph algorithms into their models. While graph computations have been studied for decades and a number of sequential (single-machine) graph algorithms are already in place, to use Pregel, for instance, one has to “think like a vertex” and recast the existing algorithms into a vertex-centric model; similarly

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when programming with other systems. The recasting is nontrivial for people who are not very familiar with the parallel models. This makes these systems a privilege for experienced users only.

Is it possible to have a system such that we can provide sequential (single-machine) graph algorithms as a whole (subject to minor changes), and it parallelizes the computation across multiple processors, without drastic degradation in either performance or functionality of the existing systems?  

**GRAPE.** To answer this question, we develop GRAPE, a parallel GRAPh Engine for graph computations such as graph traversal, graph pattern matching, graph connectivity and collaborative filtering. Using our familiar terms, we refer to a graph computation problem \( Q \) as a class of queries, and an instance \( Q \) of \( Q \) as a query of \( Q \). GRAPE differs from prior graph systems in the following.

1. **Ease of programming.** GRAPE supports a simple programming model. For a class \( Q \) of graph queries, users only need to provide (existing) sequential (incremental) algorithms for \( Q \) with minor additions. There is no need to revise the logic of the existing algorithms, and it substantially reduces the efforts to “think parallel”. This makes parallel graph computations accessible to a large group of users who know conventional graph algorithms covered in undergraduate textbooks.

2. **Termination and correctness.** GRAPE parallelizes the sequential algorithms based on a combination of partial evaluation and incremental computation. It guarantees to converge at correct answers under a monotonic condition, as long as the sequential algorithms provided are correct.

3. **Graph-level optimization.** GRAPE naturally inherits all optimization strategies available for sequential algorithms and graphs, e.g., indexing, compression and partitioning. In contrast, these strategies are hard to implement for vertex-centric programs.

4. **Scalability.** The ease of programming does not imply performance degradation compared with the state-of-the-art systems, e.g., vertex-centric Giraph [6] (Pregel) and GraphLab, and block-centric Blogel. For instance, Table 1 shows the performance of the systems for single source shortest-path queries (SSSP) over Friendster [4], a social network with 65 million users and 1.8 billion relationships (edges), using 192 processors, GRAPE outperforms Giraph, GraphLab and Blogel in both response time and communication costs (see Section 7 for more results).

| System   | Category                  | Time(second) | Communication(MB) |
|----------|---------------------------|--------------|-------------------|
| Giraph   | vertex-centric            | 434.0        | 113411.1          |
| GraphLab | vertex-centric            | 41.7         | 106756.3          |
| Blogel   | block-centric             | 112.3        | 123377.0          |
| GRAPE    | semi-auto parallelization | 24.3         | 14744.8           |

Table 1. Graph traversal on parallel systems

**A principled approach.** To see how GRAPE achieves these, we present its underlying principles. Consider a graph \( G \) that is partitioned into fragments \((F_1, \ldots, F_n)\), and distributed across \( n \) processors \((P_1, \ldots, P_n)\), where \( F_i \) resides at \( P_i \) for \( i \in [1, n] \), respectively. Given a query \( Q \in Q \) and a fragmented graph \( G \), GRAPE computes the answer \( Q(G) \) to \( Q \) in \( G \) based on the following.

**Partial evaluation.** Given a function \( f(s, d) \) and the \( s \) part of its input, partial evaluation is to specialize \( f(s, d) \) with respect to the known input \( s \) [42]. That is, it performs the part of \( f \)’s computation that depends only on \( s \), and generates a partial answer, i.e., a residual function \( f’ \) that depends on the as yet unavailable input \( d \). For each processor \( P_i \) in GRAPE, its local fragment \( F_i \) is its known input \( s \), while the data residing at other processors accounts for the yet unavailable input \( d \). GRAPE computes \( Q(F_i) \) at all processors \( P_i \)’s in parallel as partial evaluation.

**Incremental computation.** Graph computations are often iterative. If \( Q(G) \) cannot be obtained in one step by combining partial results \( Q(F_i) \), GRAPE exchanges selected partial results as messages between processors, and computes \( Q(F_i \oplus M_i) \), by treating message \( M_i \) to \( P_i \) as updates to certain status variables associated with nodes and edges in \( F_i \). It incrementally computes changes \( \Delta O_i \)

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to $Q(F_i)$ such that $Q(F_i \oplus M_i) = Q(F_i) \oplus \Delta O_i$, making maximum reuse of previous results $Q(F_i)$. Here (1) $M_i$ is a message designated to worker $P_i$, where fragment $F_i$ resides; (2) $F_i \oplus M_i$ is the abbreviation of the following steps: (a) deduce the change $\Delta F_i$ to $F_i$ from $M_i$ (we will show how to deduce the change in Section 3.2); and then (b) apply the change $\Delta F_i$ to fragment $F_i$; and (3) $Q(F_i) \oplus \Delta O_i$ is to apply the change $\Delta O_i$ to the old result $Q(F_i)$. It is to minimize the use of notations that we reload the notation $\oplus$; it will be clear from the context what operation $\oplus$ means. Incremental computation is often more efficient than recomputing $Q(F_i \oplus M_i)$ starting from scratch, since in practice $M_i$ is typically small, and so is $O_i$. Better still, it may be bounded: its cost depends only on the sizes of the changes $M_i$ to input $F_i$ and changes $\Delta O_i$ to output $Q(F_i)$, not on the size $|F_i|$ of the entire fragment $F_i$ [29, 57], minimizing unnecessary recomputation.

**Workflow.** Based on partial evaluation and incremental computation, GRAPE works as follows.

(1) **Plug.** GRAPE offers a simple programming interface as shown in Figure 1. For a class $Q$ of graph queries, developers need to specify three functions: PEval, IncEval and Assemble in the algorithm panel. PEval and IncEval are (often existing) sequential (single-machine) algorithms for $Q$, for partial evaluation and incremental computation, respectively; and Assemble is typically straightforward (see examples shortly). These can be picked from a library of graph algorithms; the only addition is a specification of messages for communication between processors.

(2) **Play.** In the configuration panel, users may pick such a specification (PEval, IncEval and Assemble) registered for $Q$, a graph $G$, a graph partition strategy and a number $n$ of processors to work with (Figure 1). Given a query $Q \in Q$ and a partitioned graph $G$, GRAPE parallelizes PEval, IncEval and Assemble across $n$ processors, and computes $Q(G)$ in three phases as shown in Figure 2.

(a) Each processor $P_i$ first executes PEval against its local fragment $F_i$, to compute partial answer $Q(F_i)$ in parallel. This facilities data-partitioned parallelism via partial evaluation.

(b) Then each processor $P_i$ may exchange partial results with other processors via synchronous message passing under BSP [65]. Upon receiving message $M_i$, processor $P_i$ incrementally computes local answer $Q(F_i \oplus M_i)$ by IncEval, operating on its local fragment $F_i$ “updated” by $M_i$. 

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**Figure 1.** Programming Interface of GRAPE

![Programming Interface of GRAPE](image-url)
(c) The incremental step iterates until no further updates \( M_i \) can be made to any \( F_i \). At this point, Assemble pulls partial answers \( Q(F_i \oplus M_i) \) from \( P_i \) for \( i \in [1, n] \) and assembles \( Q(G) \).

That is, GRAPE parallelizes sequential algorithms as a whole, and computes a simultaneous fixpoint by taking IncEval as the intermediate consequence operator. It guarantees to reach a fixpoint under a monotonic condition if the sequential algorithms are correct for \( Q \). Moreover, it minimizes iterative recomputation by using IncEval, and supports graph-level optimization on \( F_i \).

**Example 1.1.** Consider Single Source Shortest Path (SSSP), a routine graph computation problem. Given a directed graph \( G \) with edges labeled with positive weights, and a source node \( s \) in \( G \) (as a query \( Q \)), the goal is to find \( Q(G) \) including the shortest distance \( \text{dist}(s, v) \) from \( s \) to all nodes \( v \) in \( G \).

Using GRAPE, one can pick our familiar Dijkstra’s algorithm [32] as P Eval, and a bounded sequential incremental algorithm of [56, 57] as IncEval. The algorithm of [56] essentially propagates changes to vertices or edges to other vertices in the graph following an order defined on some “keys” of the affected vertices. Similarly, the algorithm by [57] handles unit changes to graphs. The only addition to GRAPE is that for each fragment \( F_i \), a variable \( \text{dist}(s, v) \) of positive numbers is declared for each node \( v \), initially \( \infty \) (except \( \text{dist}(s, s) = 0 \)). As shown in Figure 2, P Eval first computes \( Q(F_i) \); it then repeats incremental steps IncEval to compute \( Q(F_i \oplus M_i) \), where messages \( M_i \) include updated (smaller) \( \text{dist}(s, u) \) (due to new “shortcut” from \( s \)) for border nodes \( u, i.e. \), nodes with edges across different fragments. GRAPE guarantees the termination of the fixpoint computation, when no more \( \text{dist}(s, v) \) can be changed to a smaller value. At this point, Assemble takes a union of \( Q(F_i) \) as \( Q(G) \), which is provably correct (see Section 3 for details).

That is, we take sequential algorithms as P Eval, IncEval and Assemble, and specify variables \( \text{dist}(s, v) \) for updating border nodes. GRAPE takes care of details such as message passing, load balancing and fault tolerance. There is no need to recast the algorithms into a new model.

**Contributions.** We propose GRAPE, which suggests a new approach to parallelizing (existing) sequential graph algorithms, from foundation to implementation.

1. We introduce the parallel model of GRAPE, based on a fixpoint of partial evaluation and (bounded) incremental computation (Section 3). We also present the programming model of GRAPE. We show how GRAPE takes existing sequential graph algorithms as input, and parallelizes the entire algorithms, in contrast to parallelization of instructions or operators [53, 58].

2. We prove two fundamental results (Section 4): (a) Assurance Theorem guarantees that for all queries \( Q \in Q \) and graphs \( G \), GRAPE converges at correct answers \( Q(G) \) under a monotonic condition as long as its input sequential algorithms are correct, and (b) Simulation Theorem shows
that MapReduce [22], BSP (Bulk Synchronous Parallel) [65] and PRAM (Parallel Random Access Machine) [66] can be optimally simulated by GRAPE. As a consequence, algorithms developed for existing graph systems can be migrated to GRAPE without increasing complexity bounds.

(3) As examples, we show that a variety of graph computations can be readily parallelized by GRAPE (Section 5). These include graph traversal (single-source shortest path queries SSSP), graph pattern matching (via graph simulation Sim and subgraph isomorphism Subiso), connected components (CC), and collaborative filtering (CF, as an example of machine learning). We show how GRAPE easily parallelizes their sequential algorithms with minor revisions.

(4) We outline an implementation of GRAPE (Section 6). We show how GRAPE supports parallelization, message passing, fault tolerance and consistency. We also show how easily GRAPE implements graph-level optimization strategies such as indexing, compression and dynamic grouping, since the sequential algorithms directly operate on fragments of a graph, which are graphs themselves. These are not supported by the state-of-the-art vertex-centric and block-centric systems.

(5) We experimentally evaluate GRAPE (Section 7), compared with (a) Giraph, an open-source version of Pregel, (b) GraphLab, another vertex-centric system, and (c) Blogel, the fastest block-centric system we are aware of. Over real-life graphs, we find that in addition to the ease of programming, GRAPE achieves comparable performance to the state-of-the-art systems. For instance, (a) on a US road network traffic [2], GRAPE is on average 14842, 3992 and 756 times faster than Giraph, GraphLab and Blogel for SSSP, respectively, with 192 processors, due to the large diameter of the graph. (b) On other real-life graphs excluding traffic, GRAPE is on average 484, 36 and 15 times faster than Giraph, GraphLab and Blogel for SSSP, 151, 6.8 and 16 times for Sim, 149.3, 34.2 and 9.6 times for Subiso, and 4.6, 2.6 and 12.4 times for CF, respectively, when the number of processors ranges from 64 to 192. (b) In the same setting (excluding traffic), GRAPE ships on average 0.07%, 0.12% and 1.7% of the data shipped across machines by Giraph, GraphLab and Blogel for SSSP, 0.89%, 0.14% and 4.9% for Sim, 0.18%, 0.23% and 0.11% for Subiso, 5.6%, 43.3% and 3.2% for CF, respectively. When traffic is also included, GRAPE outperforms these systems by up to 6 orders of magnitude in communication cost for SSSP. (c) Incremental steps effectively reduce the cost and improve the performance of Sim by 9.6 times on average. (d) Optimization strategies for sequential algorithms remain effective for GRAPE and improve Sim by 20% on average.

Related work. This paper extends its conference version [31] as follows. (1) We provide proofs of Assurance Theorem and Simulation Theorem (Section 4). (2) We develop algorithms for graph simulation Sim, subgraph isomorphism Subiso, connected components CC, and collaborative filtering CF (Section 5). The details of the algorithms were not included in [31]. (3) We re-conduct all experiments of [31] by using larger graphs and more processors, to evaluate the scalability of GRAPE with the size of datasets and the parallel scalability with the number of processors, as well as the communication costs. We also add a COST [51] analysis of GRAPE (Section 7).

The other related work is categorized as follows.

Parallel graph systems. Several parallel models have been studied for graph computations, e.g., PRAM [66], BSP [65] and MapReduce [22]. PRAM abstracts parallel RAM access over shared memory. A large collection of parallel graph algorithms are in place for PRAM. These algorithms may need to be optimized for the shared-nothing architecture that is widely used today. MapReduce makes parallel computation accessible to a large number of users, but may not be very efficient for iterative graph computations due to its blocking nature and I/O costs. BSP has proven more appropriate for graph computations. It models parallel computations in supersteps (including local computation, communication and a synchronization barrier) to synchronize communication among workers, such that messages from one superstep are accessible in the next one. Alternatively, AP
(Asynchronous Parallel) model allows a worker to have immediate access to incoming messages. Vertex-centric models \cite{6, 49, 50} execute local computations defined at each vertex in parallel.

Several parallel graph systems have been developed under these models. Pregel \cite{50} (Giraph \cite{6}) implements BSP with vertex-centric programming, where a superstep executes a user-defined function at each vertex in parallel. GraphLab \cite{49} supports both BSP and AP with vertex-centric programming. Block-centric systems \cite{63, 71} extend vertex-centric programming to blocks, to exchange messages among blocks and reduce communication costs. Giraph++ \cite{63} supports graph-centric programming to open up subgraphs to be programmed against. Blogel \cite{71} allows blocks to have their status as a “vertex” and supports block-level communication. Nonetheless, both Giraph++ and Blogel still adopt the vertex-centric style programming paradigm.

Popular parallel graph systems also include GraphX \cite{34}, GRACE \cite{67}, GPS \cite{59}, Mizan \cite{46}, Pregel+ \cite{72} (see \cite{70} for a recent survey). GraphX \cite{34} recasts graph computation into its distributed dataflow framework as a sequence of join and group-by stages punctuated by map operations, on Spark platform. GRACE \cite{67} provides an operator-level, iterative programming model to enhance BSP with asynchronous execution. It provides a scheduler to control the order of vertex computation in a block. The system works in single-machine environment, with a focus on improving main memory utilization. GPS \cite{59} implements Pregel with extended APIs and partition strategies. It advocates an optimization strategy such that algorithms can “post” messages, for a vertex to send the same message to all of its neighbors, by partitioning the neighbors of high-degree nodes across different processors (via their mirrored nodes). Mizan \cite{46} optimizes Pregel with dynamic load balancing based on run-time monitoring of vertex computation. Pregel+ \cite{72} introduces optimized message reduction similar to GPS but with an additional cost model to trade off mirroring and message combining costs. Both Mizan and Pregel+ are based on Pregel’s model.

All these systems require recasting of existing sequential algorithms into a new model. For example, synchronous vertex programs are required by Pregel-like systems \cite{6, 46, 50, 59, 63, 72}. Sequential algorithms need to be recast to Gather-Aggregate-Scatter (GAS) vertex programs in GraphLab \cite{49}. When it comes to block-centric models \cite{63, 71}, sequential algorithms have to be recast to block-level programs that treat each subgraph as a single vertex.

This work aims to show that it is possible to parallelize existing sequential graph algorithms as a whole, without recasting the algorithms into a new model. GRAPE can simplify parallel programming and make parallel graph computations accessible to a large group of users, without drastic degradation in performance or functionality. To this end, GRAPE adopts the synchronization mechanism of BSP for its simplicity. As opposed to the prior systems, (a) GRAPE parallelizes sequential algorithms based on fixpoint computation with partial evaluation and incremental computation. (b) Following data-partitioned parallelism, given a partitioned graph, GRAPE allows workers to operate on different fragments in parallel, and exchanges among workers only the updated values of the status variables associated with border nodes. In contrast, for iterative computations, MapReduce needs to repartition graph and ship its entire state in each round \cite{50}. (c) The vertex-centric model of Pregel (synchronized) is a special case of GRAPE, when each fragment is limited to a single vertex. The communications of Pregel are via “inter-processor” messages, and a message from a node often has to go through several supersteps to reach another node. GRAPE reduces excessive messages and scheduling cost of Pregel, since communications within the same fragment are local. GRAPE also facilitates graph-level optimization methods that are hard to implement in vertex-centric systems; similarly for GraphLab (asynchronized). (d) Closer to GRAPE are block-centric models \cite{63, 71}. However, the programming interface of \cite{63} is still vertex-centric, and \cite{71} is a mix of vertex-centric and block-centric programming (V-compute and B-compute). The B-compute interface is essentially vertex-centric programming, by treating each block as a vertex. Users have to recast existing sequential algorithms into a new model. In contrast,
GRAPE takes sequential algorithms PEval and IncEval from GRAPE library, and applies them to blocks in parallel without recasting. (e) None of the prior systems uses (bounded) incremental steps to speed up iterative computations. (f) To the best of our knowledge, none of these systems provides assurance on termination and the correctness of parallel graph computations.

Partial evaluation has been studied for certain XML [19] and graph queries [29]. There has also been a host of work on incremental graph computation (e.g., [24, 29, 57]). This work makes a first effort to provide a uniform model by combining partial evaluation and incremental computation together, to parallelize sequential graph algorithms as a whole.

Parallelization of graph computations. A number of algorithms have been developed in MapReduce, vertex-centric models and others [29, 73]. In contrast, GRAPE aims to parallelize existing sequential graph algorithms, without revising their logic and work flow. Moreover, parallel algorithms for MapReduce, BSP (vertex-centric or not) and PRAM can be easily migrated to GRAPE (Section 4.2).

Prior work on automated parallelization has focused on the instruction or operator level [54, 58] by breaking dependencies via symbolic and automatic analyses. There has also been work for translating imperative code to MapReduce, e.g., word count [55]. GRAPE advocates a different approach, by parallelizing the runs of sequential graph algorithms to benefit from data-partitioned parallelism, without translation. This said, the techniques of [54, 55, 58, 75] are complementary to GRAPE.

Simulation results. Prior work has mostly focused on simulations between variants of PRAM with different memory management strategies, to characterize bounds of slowdown for deterministic or randomized solutions [38]. There has also been recent work on simulation of PRAM on MapReduce and BSP [43]. In particular, [43] defines a framework MRC for MapReduce computations and shows that a large class of PRAM algorithms can be efficiently simulated by MRC with certain restrictions. This work extends [31] by providing optimal deterministic simulation results of MapReduce, BSP and PRAM on GRAPE, adopting the notion of optimal simulations of [66].

2 PRELIMINARIES

We start with a review of basic notations.

Graphs. We consider graphs \( G = (V, E, L) \), directed or undirected, where (1) \( V \) is a finite set of nodes; (2) \( E \subseteq V \times V \) is a set of edges; (3) each node \( v \) in \( V \) (resp. edge \( e \) in \( E \)) carries \( L(v) \) (resp. \( L(e) \)), indicating its content, as found in social networks, knowledge bases and property graphs.

We use two notions of subgraphs. A graph \( G' = (V', E', L') \) is called a subgraph of \( G \) if \( V' \subseteq V \), \( E' \subseteq E \), and for each node \( v \) in \( V' \) (resp. edge \( e \) in \( E' \)), \( L'(v) = L(v) \) (resp. \( L'(e) = L(e) \)). A subgraph \( G' \) is said to be induced by \( V' \) if \( E' \) consists of all the edges in \( G \) whose endpoints are both in \( V' \).

Partition strategy. Given a graph \( G \) and a number \( m \), a graph partition strategy \( \mathcal{P} \) partitions \( G \) into fragments \( \mathcal{F} = (F_1, \ldots, F_m) \) such that each \( F_i = (V_i, E_i, L_i) \) is a subgraph of \( G \), \( E = \bigcup_{i \in [1, m]} E_i \), \( V = \bigcup_{i \in [1, m]} V_i \), and \( F_i \) resides at processor \( P_i \) for \( i \in [1, m] \). In vertex partition (a.k.a. edge-cut) [12, 18]), a cut edge from fragment \( F_i \) to \( F_j \) has a copy in each of \( F_i \) and \( F_j \). Denote by

- \( F_i.1 \) (resp. \( F_i.0' \)) the set of nodes \( v \) in \( V_i \) such that there exists an edge \((v', v)\) from \((v, v')\) to a node \( v' \) in \( F_j \) \((i \neq j)\);
- \( F_i.O \) (resp. \( F_i.I' \)) the set of nodes \( v' \) in some \( F_j \) \((i \neq j)\) such that there exists an edge \((v, v')\) from \((v', v)\) to \( v \) in \( V_i \); and
- \( \mathcal{F}.O = \bigcup_{i \in [1, m]} F_i.O \), \( \mathcal{F}.O' = \bigcup_{i \in [1, m]} F_i.O' \), \( \mathcal{F}.I = \bigcup_{i \in [1, m]} F_i.I \), \( \mathcal{F}.I' = \bigcup_{i \in [1, m]} F_i.I' \).
We refer to those nodes in \( F_i \cup F_j \cup O \) as the border nodes of fragment \( F_i \) with respect to partition strategy \( \mathcal{P} \). Note that \( \mathcal{F}.I = \mathcal{F}.O \) and \( \mathcal{F}.I' = \mathcal{F}.O' \).

In edge partition (a.k.a. vertex-cut) [47], the cut vertices are called entry vertices and exit vertices for the partitions, which correspond to the sets \( \mathcal{F}.O \cup \mathcal{F}.I' \) and \( \mathcal{F}.I \cup \mathcal{F}.O' \), respectively. In general, a border node is a vertex that relates to vertices or edges in two different fragments.

The fragmentation graph \( \mathcal{G}_{\mathcal{P}} \) of \( G \) via \( \mathcal{P} \) is an index such that given each border node \( v \) in \( F_i.I \) (resp. \( F_i.O' \) \((i \in [1, m])\), \( \mathcal{G}_{\mathcal{P}}(v) \) retrieves a set of \( \{j | v \in F_j.O\} \) (resp. \( \{j | v \in F_j.I'\} \)). As will be seen shortly, we will make use of \( \mathcal{G}_{\mathcal{P}} \) to deduce the directions of messages.

The notations of this paper are summarized in Table 2.

| symbols | notations |
|---------|-----------|
| \( \mathcal{Q} \) | a class of graph queries |
| \( Q \) | a query \( Q \in \mathcal{Q} \) |
| \( G \) | graph, directed or undirected |
| \( P \) | graph partition strategy |
| \( G_{\mathcal{P}} \) | the fragmentation graph of \( G \) via partition strategy \( \mathcal{P} \) |
| \( F_i \) | the \( i \)-th fragment of graph \( G \) via partition strategy \( \mathcal{P} \) |
| \( V_i, E_i \) | vertex set and edge set of fragment \( F_i \), respectively |
| \( I \) | fragmentation \((F_1, \ldots, F_n)\) of graph \( G \) |
| \( O \) | messages designated to worker \( F_i \) |
| \( F_i \oplus O \) | fragment \( F_i \) updated with message \( O \) |

Table 2. Notations

3 PROGRAMMING WITH GRAPE

Below we first introduce the parallel model of GRAPE. We then show how to program with GRAPE. Following BSP [65], GRAPE works with a coordinator \( P_0 \) and a set of \( m \) workers \( P_1, \ldots, P_m \).

3.1 The Parallel Model of GRAPE

Given a graph partition strategy \( \mathcal{P} \) and sequential algorithms PEval, IncEval and Assemble for a class \( \mathcal{Q} \) of graph queries, GRAPE parallelizes the computations as follows. It first partitions graph \( G \) into fragments \( \mathcal{F} = (F_1, \ldots, F_n) \) with strategy \( \mathcal{P} \), and distributes the fragments across \( m \) shared-nothing virtual workers \( (P_1, \ldots, P_m) \). It maps \( m \) virtual workers to \( n \) physical workers such that fragment \( F_i \) resides at worker \( P_i \) for \( i \in [1, m] \). When \( n < m \), multiple virtual workers mapped to the same worker share memory. It also constructs fragmentation graph \( \mathcal{G}_{\mathcal{P}} \). Note that graph \( G \) is partitioned once for all queries \( Q \in \mathcal{Q} \) posed on graph \( G \).

**Parallel model.** Given a query \( Q \in \mathcal{Q} \), GRAPE computes answer \( Q(G) \) to \( Q \) in the partitioned graph \( G \), as shown in Figure 2. Upon receiving \( Q \) at coordinator \( P_0 \), GRAPE posts the same query \( Q \) to all the workers. To simplify the discussion, here we adopt synchronous message passing following BSP [65]. We will show how GRAPE implements point-to-point communication in Section 6. Furthermore, GRAPE also works under asynchronous parallel models [27].

Its parallel computation consists of the following three phases.

1. **Partial evaluation (PEval).** In the first superstep, upon receiving query \( Q \), each worker \( P_i \) computes partial result \( Q(F_i) \) locally at its fragment \( F_i \) using PEval, in parallel (for \( i \in [1, m] \)). It also identifies and initializes a set of update parameters for each \( F_i \) that records the status of certain nodes, e.g., border nodes. At the end of the process, it generates a message from the update parameters at each \( P_i \), and sends it to coordinator \( P_0 \) (see Section 3.2 for update parameters).
We next elaborate the three functions in a \[\text{PIE}\] program. We now introduce the programming model of \[\text{GRAPE}\].

Each superstep consists of two steps, one at the coordinator \(P_0\) and the other at the workers.

(2.a) \textbf{Coordinator}. Coordinator \(P_0\) checks whether for all \(i \in [1, m]\), worker \(P_i\) is inactive, i.e., \(P_i\) is done with its local computation and there exists no pending message designated for \(P_i\). If so, \[\text{GRAPE}\] invokes \[\text{Assemble}\] and terminates (see below). Otherwise, \(P_0\) composes a message \(M_i\) by aggregating messages from the last superstep (see details shortly), sends \(M_i\) to worker \(P_i\) for \(i \in [1, m]\), and triggers the next superstep.

(2.b) \textbf{Workers}. Upon receiving message \(M_i\), worker \(P_i\) \textit{incrementally} computes \(Q (F_i \oplus M_i)\) with \[\text{IncEval}\], by treating \(M_i\) as updates, in parallel for all \(i \in [1, m]\). Here \(F_i \oplus M_i\) denotes the fragment \(F_i\) that is updated with message \(M_i\), i.e., \(F_i\) after its update parameters are changed with the values in \(M_i\). At the end of the process, \[\text{IncEval}\] automatically finds the changes to the update parameters in each \(F_i\), and sends the changes as a message to coordinator \(P_0\) (see Section 3.3 for details).

\[\text{GRAPE}\] supports data-partitioned parallelism by \textit{partial evaluation} on local fragments, in parallel by all workers. Its \textit{incremental step} (2.b) speeds up iterative graph computations by reusing the partial results from the last superstep, to minimize unnecessary recomputation.

(3) \textbf{Termination (Assemble)}. The coordinator \(P_0\) decides to terminate the process if there exists no more change to any update parameters (see (2.a) above). If so, \(P_0\) pulls partial results from all workers, and computes \(Q (G)\) by invoking \[\text{Assemble}\]. It returns query answer \(Q (G)\).

We will show in Section 4 that the parallel process converges at correct answers under a monotonic condition as long as the sequential algorithms \[\text{PEval}\], \[\text{IncEval}\] and \[\text{Assemble}\] are correct; moreover, the simple parallel model does not lose expressive power.

\[\text{3.2 PEval: Partial Evaluation}\]

We now introduce the programming model of \[\text{GRAPE}\]. \[\text{GRAPE}\] provides a programming interface for users to extend (existing) sequential algorithms with message declarations. \[\text{GRAPE}\] registers the algorithms as stored procedures in its API library (Figure 1), and maps them to a query class \(Q\).

More specifically, for a class \(Q\) of graph queries, one only needs to provide three core functions \[\text{PEval}\], \[\text{IncEval}\] and \[\text{Assemble}\] (see the Plug Panel in Figure 1), referred to as a \textit{PIE program}. These are conventional (existing) sequential algorithms, and can be picked from Library API of \[\text{GRAPE}\].

We next elaborate the three functions in a \textit{PIE} program.

Function \[\text{PEval}\] takes a query \(Q \in Q\) and a fragment \(F_i\) of \(G\) as input, and computes partial answers \(Q (F_i)\) at worker \(P_i\) in parallel for all \(i \in [1, m]\). It may be any existing sequential algorithm for \(Q\). One only needs to extend it with the following additions:

- \textit{partial result} kept in a designated variable; and
- \textit{message specification} as its interface to \[\text{IncEval}\].

Communication among workers is conducted via message passing. Messages are defined in terms of \textit{update parameters} of each fragment \(F_i\) as follows.

(1) \textbf{Message preamble}. Function \[\text{PEval}\] (a) declares \textit{status variables} \(\bar{x}\) associated with vertices and edges for each fragment \(F_i\), and (b) specifies a set \(C_i\) of nodes and edges relative to \(F_i, I\) or \(F_i, O'\) w.r.t. each fragment \(F_i\). The status variables associated with \(C_i\) are denoted by \(C_i, \bar{x}\), and are referred to as the \textit{update parameters} of \(F_i\). The variables are declared and initialized in \[\text{PEval}\]. At the end of \[\text{PEval}\], it sends the values of \(C_i, \bar{x}\) to coordinator \(P_0\).

Intuitively, variables in \(C_i, \bar{x}\) are the candidates to be updated by incremental steps. In other words, messages \(M_i\) to worker \(P_i\) are \textit{updates} to the values of variables in \(C_i, \bar{x}\).
More specifically, in GRAPE, $C_i$ is specified by an integer $d$ and $S$, where $S$ is either $F_i.I$ or $F_i.O'$. That is, $C_i$ is the set of nodes and edges within $d$-hops of nodes in $S$. In most cases $d = 0$ and $C_i$ is $F_i.I$ or $F_i.O'$. However, in some applications one needs $d \geq 0$, e.g., subgraph isomorphism (SubIso, see Section 5.1). In such cases $C_i$ may include nodes and edges from other fragments $F_j$ of $G$.

A message $M_i$ is a set of key-value pairs $(x, val)$, where $x$ is a status variable declared in $C_i,.x$ and val is its value. GRAPE supports arbitrarily typed status variables, e.g., val of $M_i$ can be a numeric value (e.g., in the algorithm for SSSP in Example 3.1), a multi-set of tuples $(r, key, value)$ (in the simulation of MapReduce in the proof of Theorem 4.2), or even a user-defined structure (a class).

(2) Message segment. PEval specifies function aggregateMsg, to resolve conflicts when multiple messages from different workers attempt to assign different values to the same update parameter (variable). When such a strategy is not provided, GRAPE picks a default exception handler.

(3) Message grouping. GRAPE deduces updates to $C_i,.x$ for $i \in [1, m]$, and treats them as messages exchanged among workers. More specifically, at coordinator $P_0$, GRAPE identifies and maintains $C_i,.x$ for each worker $P_i$. Upon receiving messages from $P_i$’s, GRAPE works as follows.

(a) Identifying $C_i$. It deduces $C_i$ for $i \in [1, m]$ by referencing fragmentation graph $G_P$, and $C_i$ remains unchanged in the entire process. It maintains update parameters $C_i,.x$ for $F_i$.

(b) Composing $M_i$. For messages from each $P_i$, GRAPE does the following:

(i) it identifies variables in $C_i,.x$ with changed values;

(ii) it deduces the designations $P_j$ of the messages by referencing the fragmentation graph $G_P$; if $P$ is edge-cut, the variable tagged with a node $v$ in $F_i.I$ will be sent to worker $P_j$ if $v$ is in $F_j.O$ (i.e., if $j$ is in $G_P(v)$); similarly for $v$ in $F_i.O'$; if $P$ is vertex-cut, it identifies nodes shared by $F_i$ and $F_j$ ($i \neq j$); and

(iii) it combines all changed variable values designated to $P_j$ into a single message $M_j$, and sends $M_j$ to worker $P_j$ in the next superstep for all $j \in [1, m]$.

If a variable $x$ is assigned a set $S$ of values from different workers, function aggregateMsg is applied to $S$ to resolve the conflicts, and its result is taken as the value of $x$. When a node $v$ has copies $v_i \in F_i$ and $v_j \in F_j$ residing in different fragments, e.g., when $v$ is a border node in $F_i.O \cap F_j.I$ ($i \neq j$), $v_i,.x$ and $v_j,.x$ are treated as the same status variable $x$ and are assigned the same value.

These are automatically conducted by GRAPE, which minimizes communication costs by passing only updated variable values. To reduce the workload at the coordinator, alternatively each worker may maintain a copy of $G_P$ and deduce the designation of its messages in parallel (see Section 6).

Example 3.1. We show how GRAPE parallelizes SSSP (see Example 1.1). Consider a directed graph $G = (V, E, L)$ in which for each edge $e$, $L(e)$ is a positive number. The length of a path $(v_0, \ldots, v_k)$ in $G$ is the sum of $L(v_{i-1}, v_i)$ for $i \in [1, k]$. For a pair $(s, v)$ of nodes, denote by dist$(s, v)$ the shortest distance from $s$ to $v$, i.e., the length of a shortest path from $s$ to $v$. Given graph $G$ and a node $s$ in $V$, GRAPE computes dist$(s, v)$ for all nodes $v \in V$. It adopts edge-cut partition [18]. It deduces $F_i.O$ by referencing $G_P$, and stores $F_i.O$ at each fragment $F_i$.

As shown in Figure 3, PEval (lines 1-14) is verbally identical to Dijkstra’s sequential algorithm [32]. The only changes are message preamble and segment (underlined). It declares an integer variable dist$(s, v)$ for each node $v$, initially $\infty$ (except dist$(s, s) = 0$). It specifies min as aggregateMsg to resolve conflicts: if there are multiple values for the same dist$(s, v)$, the smallest value is taken by the linear order on integers. The update parameters are $C_i,.x = \{\text{dist}(s, v) \mid v \in F_i.O\}$.

At the end of its process, PEval sends $C_i,.x$ to coordinator $P_0$. At $P_0$, GRAPE maintains dist$(s, v)$ for all $v \in F.0 = F.I$. Upon receiving messages from all workers, it takes the smallest value
for each \(\text{dist}(s, v)\). It finds those variables with smaller values, deduces their destinations \(P_j\) by referencing fragmentation graph \(G_P\), groups them into messages \(M_j\), and sends \(M_j\) to worker \(P_j\). □

### 3.3 IncEval: Incremental Evaluation

Given query \(Q\), fragment \(F_i\), partial results \(Q(F_i)\) and message \(M_i\) (updates to \(C_i, \bar{x}\)), IncEval computes \(Q(F_i \oplus M_i)\) incrementally, making maximum reuse of the computation of \(Q(F_i)\) in the last round. Here \(F_i \oplus M_i\) denotes \(F_i\) updated with \(M_i\). Each time after IncEval is executed, GRAPE treats \(F_i \oplus M_i\) and \(Q(F_i \oplus M_i)\) as \(F_i\) and \(Q(F_i)\), respectively, for the next round of incremental computation.

Function IncEval can be any existing sequential incremental algorithm for \(Q\). It shares the message preamble of PEval. At the end of the process, it identifies changed values to \(C_i, \bar{x}\) at each fragment \(F_i\), and sends the changes as messages to \(P_0\). Upon receiving the messages at coordinator \(P_0\), GRAPE composes these messages as described in 3(b) in Section 3.2.

**Boundedness.** Graph computations are typically iterative. GRAPE reduces the costs of iterative computations by promoting bounded incremental algorithms for IncEval.

Consider an incremental algorithm IncEval for \(Q\). Given \(G, Q \in Q, Q(G)\) and updates \(M\) to \(G\), it computes \(\Delta O\) such that \(Q(G \oplus M) = Q(G) \oplus \Delta O\), where \(\Delta O\) denotes changes to the old output \(Q(G)\). It is said to be bounded if its cost can be expressed as a function in the size of \(|\text{CHANGED}| = |M| + |\Delta O|\), i.e., the size of changes in the input and output [28, 57]. Intuitively, \(|\text{CHANGED}|\) represents the updating costs inherent to the incremental problem for \(Q\) itself. For a bounded IncEval, its cost is determined by \(|\text{CHANGED}|\), not by the size \(|F_i|\) of entire \(F_i\), no matter how big \(|F_i|\) is. That is, it reduces computation on possibly big \(F_i\) to smaller data bounded by \(O(|\text{CHANGED}|)\).

**Example 3.2.** Continuing with Example 3.1, we provide IncEval in Figure 4. It is the sequential incremental algorithm for SSSP developed in [56, 57], in response to changed \(\text{dist}(s, v)\) for \(v\) in \(F_i.I\) (here message \(M_i\) includes changes to \(\text{dist}(s, v)\) for \(v \in F_i.I\) deduced from \(G_P\)). Using a queue \(\text{Que}\),
Input: $F_i(V_i, E_i, L_i)$, partial result $Q(F_i)$, message $M_i$.  
Output: $Q(F_i \oplus M_i)$.

1. initialize priority queue $Que$;
2. for each $dist(s, v)$ in $M$ do
3.   $Que$.addOrAdjust($v$, $dist(s, v)$);
4. while $Que$ is not empty do
5.   $u := Que$.pop(); /* pop vertex with minimum distance*/
6.   for each child $v$ of $u$ do /* only $v$ that still has not been visited */
7.     $alt := dist(s, u) + L_i(u, v)$;
8.     if $alt < dist(s, v)$ then
9.       $dist(s, v) := alt$;
10. $Q(F_i) := \{dist(s, v) | v \in V_i\}$

Message segment: $M_i = \{dist(s, v) | v \in F_i.O, dist(s, v)$ decreased\};

Fig. 4. IncEval for SSSP

it starts with $M_i$, propagates the changes to affected area, and updates the distances (see [56, 57] for details). The partial result is now the revised distances (line 11).

At the end of the process, IncEval sends to coordinator $P_0$ updated values of those status variables in $C_i, \bar{x}$, as in PEval. It applies aggregateMsg min to resolve conflicts.

The changes to the algorithm of [56, 57] are underlined in Figure 4. Following [56, 57], one can show that IncEval is bounded: its cost is determined by the sizes of "updates" $|M_i|$ and the changes to the output. This reduces the cost of iterative computation of SSSP (the while and for loops).

Note that IncEval only needs to deal with changes $M_i$, e.g., changes to $dist(s, v)$ for $v \in F_i.I$ in Example 3.2. That is, changes are restricted to the update parameters, rather than generic updates.

3.4 Assemble Partial Results

Function Assemble takes partial results $Q(F_i \oplus M_i)$ and fragmentation graph $G_f$ as input, and combines $Q(F_i \oplus M_i)$ to get complete query answer $Q(G)$. It is triggered when no more changes can be made to update parameters $C_i, \bar{x}$ for any $i \in [1, m]$.

Example 3.3. Continuing with Example 3.2, function Assemble (not shown) for SSSP takes $Q(G) = \bigcup_{i \in [1, n]} Q(F_i)$, the union of the shortest distance for each node in each $F_i$.

The GRAPE process terminates with correct $Q(G)$. Indeed, the updates to $C_i, \bar{x}$ are "monotonic": the value of $dist(s, v)$ for each node $v$ decreases or remains unchanged. There are finitely many such variables. Furthermore, $dist(s, v)$ is the shortest distance from $s$ to $v$, as warranted by the correctness of the sequential algorithms of [32, 56, 57] (i.e., PEval and IncEval).

Putting these together, one can see that a PIE program parallelizes a graph query class $Q$ provided with a sequential algorithm (PEval) and a sequential incremental algorithm (IncEval) for $Q$. Moreover, Assemble is typically a straightforward algorithm. A large number of sequential (incremental) algorithms are already in place for various $Q$, after decades of study of graph computations. Thus GRAPE is promising for making parallel graph computations accessible to a large group of users.

Remark. Observe the following about PEval, IncEval, and Assemble.

(1) There have been methods for incrementalizing algorithms, to get incremental algorithms from their batch counterparts [11, 24]. Moreover, incremental algorithm IncEval only needs to deal with changes to status variables (update parameters), not necessarily generic updates (although to focus on the main idea, we present IncEval using the familiar notion of incremental graph algorithms).
Such changes are aggregated by function \( f_{aggr} \) and depend on how \( f_{aggr} \) is defined. Hence it is often not hard to develop IncEval by revising a batch algorithm in response to changes to update parameters, as will be shown by the case of CC (connected components) in Section 5.2.

(2) Incremental IncEval speeds up iterative computations by minimizing unnecessary recomputation of \( Q(F_i) \) at each worker \( P_i \), no matter whether IncEval is bounded or not. Indeed, boundedness is not the only criterion for the effectiveness of incremental algorithms. Alternative performance guarantees for incremental graph algorithms have been developed, such as semi-boundedness [28], localizable incremental algorithms and relative boundedness [24].

(3) In contrast to existing graph systems, GRAPE parallelizes sequential algorithms PEval and IncEval as a whole, with additional declaration of message segment (PEval). As a result, users do not have to “think like a vertex” [49, 50, 63, 71] when programming. As opposed to vertex-centric and block-centric systems, GRAPE runs sequential algorithms on entire fragments. Moreover, IncEval employs incremental evaluation to reduce cost, which is a unique feature of GRAPE.

(4) GRAPE aims to help users develop parallel programs, especially those who are more familiar with conventional sequential programming. This said, users of GRAPE still need to know the domain knowledge to design update parameters and aggregate functions.

4 FOUNDATION OF GRAPE

We next present fundamental results underlying GRAPE. We first identify a condition under which a PIE program guarantees to converge at correct answers under GRAPE (Section 4.1). We then demonstrate the expressive power of GRAPE by simulating BSP, MapReduce and PARM (Section 4.2).

4.1 Correctness of Parallel Model

Consider a partition strategy \( \mathcal{P} \) and a PIE program \( \rho \) for a class \( Q \) of graph queries, where \( \rho \) consists of functions PEval, IncEval and Assemble. Given a query \( Q \in Q \), a graph \( G \) and a natural number \( m \), the GRAPE parallelization of \( \rho \) can be modeled as a simultaneous fixpoint operator defined on \( m \) fragments. More specifically, it starts with PEval for partial evaluation, and conducts incremental computation by taking IncEval as the intermediate consequence operator:

\[
R_0^i = \text{PEval}(Q, F_0^i[\bar{x}_i]),
R_{i+1}^i = \text{IncEval}(Q, R_i^r, F_i[\bar{x}_i], M_i),
\]

where for \( i \in [1, m] \), \( r \) indicates a superstep; \( F_i^0 \) is the fragment \( F_i \) assigned to worker \( P_i \) by the partition of \( G \) via \( \mathcal{P} \); \( F_i^r[\bar{x}_i] \) is fragment \( F_i \) at the end of superstep \( r \) carrying update parameters \( C_i, \bar{x}_i; M_i \) indicates changes to \( C_i, \bar{x}_i \) (via message); and \( R_i^r \) denotes partial results (including values of \( C_i, \bar{x}_i \)) computed at fragment \( F_i \) after the \((r + 1)\)-th superstep. The computation proceeds until it reaches \( r_0 \) such that \( R_i^{r_0} = R_i^{r_0+1} \). At this point, Assemble\((R_1^{r_0}, \ldots, R_m^{r_0})\) is computed and returned.

Note that the computation does not reach a fixpoint as long as update parameters \( C_i, \bar{x}_i \) keep changing. This is consistent with the parallel model of GRAPE (Section 3.1).

There has been a large body of work on fixpoint computation, to study (a) whether a fixpoint computation converges [20, 35, 52, 74]; and (b) how to accelerate fixpoint computation [35, 40, 60, 69]. In this paper, we mainly focus on (a). Issue (b) has been addressed in [27], which is based on GRAPE.

As an example, below we identify one convergence guarantee for the simple parallel model as a sufficient condition. We start with some notations.

(1) We say that PIE program \( \rho \) terminates under GRAPE with \( \mathcal{P} \) if for all queries \( Q \in Q \) and all graphs \( G \), there always exists \( r_0 \) such that at superstep \( r_0 \), \( R_i^{r_0} = R_i^{r_0+1} \) for all \( i \in [1, m] \).

(2) We say that a PIE program \( \rho \) with PEval, IncEval and Assemble is correct for \( Q \) w.r.t. \( \mathcal{P} \) if for all
queries $Q \in Q$ and all graphs $G$ fragmented into $F_1, \ldots, F_m$ with $P$, Assemble($R^t_i, \ldots, R^t_m$) = $Q(G)$ at any superstep $r$ when update parameters in $R^t_i (i \in [1, m])$ have the same values as in $R^{t-1}_i$, where $Q(G)$ is the answer to $Q$ in $G$, and $R^t_i$ is the partial result computed at $F_i$ after the $(r+1)$-th superstep.

We say that GRAPE correctly parallelizes $\rho$ with partition strategy $P$ if for all queries $Q \in Q$ and all graphs $G$, $\rho$ always terminates under GRAPE with $P$ and returns $Q(G)$.

(3) We say that PEval and IncEval satisfy the monotonic condition w.r.t. partition strategy $P$ if for graphs $G$ and every variable $x \in C_i, \bar{x}$ for $i \in [1, m]$, (a) the values of $x$ are from a finite set computed from values in the active domain of $G$ (i.e., the constants in $G$); and (b) there exists a partial order $\preceq_{p_x}$ on the values of $x$ such that IncEval decreases $x$ in the order of $p_x$.

Intuitively, condition (a) above says that $x$ draws values from a finite domain, and condition (b) says that $x$ is updated “monotonically” following $p_x$. These ensure that PIE programs with PEval and IncEval terminate under GRAPE with $P$. For instance, dist$(s, v)$ in Example 3.1 can only be changed in the decreasing order (i.e., it is computed by function min for aggregateMsg of IncEval in the active domain of $G$), and hence PEval and IncEval for SSSP satisfy the monotonic condition.

We next provide a condition that warrants the correctness of GRAPE parallelization.

**Theorem 4.1 [Assurance Theorem]:** Consider a PIE program $\rho$ with PEval, IncEval and Assemble for a class $Q$ of graph queries. GRAPE correctly parallelizes $\rho$ with a graph partition strategy $P$ if

(a) PEval and IncEval satisfy the monotonic condition w.r.t. $P$, and

(b) $\rho$ with PEval, IncEval and Assemble is correct for $Q$ w.r.t. $P$.

More specifically, (1) under the monotonic condition, the PIE program $\rho$ guarantees to terminate under GRAPE and better yet, (2) it converges at correct answer $Q(G)$ for all queries $Q \in Q$ and all graphs $G$ as long as the sequential algorithms PEval, IncEval and Assemble of $\rho$ are correct for $Q$. In other words, condition (a) guarantees termination of a PIE program under GRAPE, and conditions (a) and (b) put together guarantee the correctness of a PIE program under GRAPE.

**Proof.** We show the correctness of Theorem 4.1 by analyzing the computations of a PIE program. Consider any run of a PIE algorithm depicted in Fig. 5. Observe the following.

(1) **Termination.** Under the monotonic condition of Theorem 4.1, we have that $\ldots \preceq_{p_x} R^{t-1}_i \preceq_{p_x} \ldots \preceq_{p_x} R^t_i \preceq_{p_x} R^0_i$ for all $i \in [1, m]$. Since $R^0_i, R^1_i, \ldots, R^{t+1}_i, \ldots$ are from a finite domain, we know that there exists a number $n$ such that $R^{t+1}_i = R^t_i$ for all $i \in [1, m]$ and $t \geq n$. That is, $\rho$ terminates.

(2) **Correctness.** From the argument above it follows that $\rho$ must terminate at some superstep $r_0$. Hence, by condition (b), Assemble($R^0_i, \ldots, R^0_m$) = $Q(G)$, i.e., $\rho$ computes $Q(G)$.

**Remark.** Observe the following.

(1) The fixpoint computation model does not reduce the expressive power of GRAPE. Indeed, (a) fixpoint computation has sufficient expressive power; many data mining and machine learning algorithms can be modeled as fixpoint computations [60, 69]. (b) We can conduct any computation in PEval and IncEval, and hence by GRAPE. We will see a formal characterization in Section 4.2.

(2) The monotonic condition is a sufficient condition for GRAPE computations to converge, but
it is not a necessary condition. Indeed, there has been a large body of work on convergence, e.g., [35, 40, 60, 69], from which other characterizations can be deduced.

(3) It does not mean that only algorithms satisfying the monotonic condition can be parallelized in GRAPE. As will be shown by Theorem 4.2, any MapReduce algorithm can be migrated to GRAPE without extra complexity, and not all MapReduce algorithms are monotonic. The monotonicity is just a sufficient condition under which users do not have to worry about convergence.

4.2 The Expressivity of GRAPE

We next show that the simple parallel model of GRAPE does not imply degradation in the expressivity. As a result, GRAPE can readily switch to other parallel models without extra complexity.

Following [66], we say that a parallel model $M_1$ can *optimally simulate* model $M_2$ if there exists a compilation algorithm that transforms any program with cost $C$ on $M_2$ to a program with cost $O(C)$ on $M_1$. The cost includes computational and communication costs. For GRAPE, these are measured by the running time of PEval, IncEval and Assemble on all the processors, and by the total size of the messages passed among all the processors in the entire process.

We show that GRAPE optimally simulates popular parallel models MapReduce [22], BSP [65] and PRAM [66]. Note that GRAPE parallelization is modeled as a simultaneous fixpoint computation. Moreover, GRAPE is a BSP system under the following constraints: (1) in each round of computation, GRAPE runs the same function PEval or IncEval, while other parallel systems may run different user-defined functions in different rounds (e.g., MapReduce); and (2) GRAPE only allows the status variables of the same vertex in different fragments to be exchanged, while there is no such restriction in some other parallel systems. We show that despite these restrictions, GRAPE does not degrade in expressive power, i.e., it is as powerful as MapReduce, BSP and PRAM.

As a consequence of the result, all algorithms developed for graph systems based on these models can be migrated to GRAPE without increasing complexity bounds, including Pregel [50], GraphX [34], Giraph++ [63] and Blogel [71]. The result below is stronger than its counterpart in [31] in that it does not use key-value pairs (messages) in the simulation (see electronic appendix for proof).

**Theorem 4.2 [Simulation Theorem]:**

1. All BSP algorithms with $n$ workers in $k$ supersteps can be optimally simulated on GRAPE with $n$ workers in $k$ supersteps;
2. All MapReduce programs using $n$ processors can be optimally simulated by GRAPE using $n$ processors; and
3. All CREW PRAM algorithms using $O(P)$ total memory, $O(P)$ processors and $t$ time can be run in GRAPE in $O(t)$ supersteps using $O(P)$ processors with $O(P)$ memory.

**Remark.** (1) Theorem 4.2 aims to show the expressive power of GRAPE, e.g., all MapReduce algorithms can be migrated to GRAPE without increasing the complexity bounds. Nonetheless, it is possible that some simulated applications are not efficient in practice, due to a possible large constant in the simulation complexity $O(C)$ (see the proof of Theorem 4.2 in the electronic appendix).

(2) As indicated by Theorem 4.2, all parallel algorithms for MapReduce, BSP and PRAM are also supported by GRAPE. Moreover, those graph computations that have effective (e.g., bounded) incremental algorithms can be accelerated by GRAPE.

(3) Compared with the vertex-centric model, the ability to run sequential algorithms over an entire fragment has several benefits. One of them is that it can reduce the number of supersteps, as demonstrated by SSSP. This is because within the fragment each worker can do some computation that would have required extra supersteps in a vertex-centric system like Pregel. This is analogous...
We start with graph pattern matching, which is commonly used in social media marketing [30], social network analysis [25] and knowledge base expansion [23], among other things.

5.1 Graph Pattern Matching

We study two semantics of graph pattern matching. We adopt edge-cut [12, 18] in this section unless stated otherwise. Under vertex-cut [47] and other graph partition strategies, PIE programs can be developed similarly.

Graph simulation. A graph $G = (V, E, L)$ matches a pattern $Q = (V_Q, E_Q, L_Q)$ via graph simulation if there exists a binary relation $R \subseteq V_Q \times V$ such that:

(a) for each query node $u \in V_Q$, there exists a node $v \in V$ such that $(u, v) \in R$, and
(b) for each pair $(u, v) \in R$, (i) $L_Q(u) = L(v)$, and (ii) for each query edge $(u, u') \in E_Q$, there exists an edge $(v, v')$ in graph $G$ such that $(u', v') \in R$.

For $(u, v) \in R$, we refer to $v$ as a match of $u$. It is known that if $G$ matches $Q$, then there exists a unique maximum relation [39], referred to as $Q(G)$. If $G$ does not match $Q$, then $Q(G)$ is the empty set. Moreover, $Q(G)$ can be computed in $O((|V_Q| + |E_Q|)(|V| + |E|))$ time [25, 39].

Graph pattern matching via graph simulation is stated as follows.

○ Input: A directed graph $G$ and a graph pattern $Q$.
○ Output: The unique maximum relation $Q(G)$.

We next show how GRAPE parallelizes graph simulation.

(1) PEval. GRAPE takes the sequential algorithm of [39] as PEval to compute $Q(F_1)$ in parallel. Its message preamble declares a Boolean status variable $x_{(u, v)}$ for each query node $u$ in $V_Q$ and each node $v$ in $F_1$, indicating whether $v$ matches $u$, initialized true. It takes $F_1, I$ as candidate set $C_I$. 

ACM Trans. Datab. Syst., Vol. 0, No. 0, Article 38. Publication date: 2000.
Input: \( Q = (V_Q, E_Q, L_Q) \), \( F_i = (V_i, E_i, L_i) \) (equally for \( G \)).

Output: Maximum match relation sim.

Message preamble: /*candidate set \( C_i \) is \( F_i, I' \)*/

for each node \( u \) in \( V_Q \) and \( v \) in \( V_i \) a Boolean \( x(u, v) := \text{true} \);

/*sequential algorithm for graph simulation (pseudo-code)*/

1. \( V_i := (V_i \setminus F_i, I') \cup F_i, O \);
2. \( E_i := E_i \setminus \{(u, v) \in E_i | u \in F_i, I' \land v \in F_i, I \} \);
3. for each \( u \) in \( V_Q \) do /* Initialization */
4.   if \( \text{post}(u) = \emptyset \) then
5.     \( \text{sim}(u) := \{v \in V_i | L_Q(u) = L_i(v)\} \);
6.   else \( \text{sim}(u) := \{v \in V_i | L_Q(u) = L_i(v) \land \text{post}(v) \neq \emptyset\} \);
7.   remove(\( u \)) := \( \text{pre}(V_i) \setminus \text{pre}(\text{sim}(u)) \);
8.   for each \( v \in V_i \setminus \text{sim}(u) \) do \( x(u, v) := \text{false} \);
9. while there exists \( u \in V_Q \) such that \( \text{remove}(u) \neq \emptyset \) do
10.  for each \( u' \in \text{pre}(u) \) do /* Refinement */
11.     for each \( w \) in \( \text{remove}(u) \) do
12.       if \( w \in \text{sim}(u') \) then
13.         \( \text{sim}(u') := \text{sim}(u') \setminus \{w\} \); \( x(u', v) := \text{false} \);
14.         for each \( w' \in \text{pre}(w) \) do
15.           if \( \text{post}(w') \cap \text{sim}(u') = \emptyset \) then
16.             remove(\( u' \)) := \( \text{remove}(u') \cup \{w'\} \);
17.             remove(\( u \)) := \( \emptyset \);
18.   \( Q(F_i) := \text{sim} \);

Message segment: \( M_i := \{x(u, v) | u \in V_Q \land v \in F_i, I\} \);

aggregateMsg = \( \min(x(u, v)) \);

Fig. 6. PEval for graph simulation in GRAPE

Before giving the details of PEval, we first review the algorithm in [39]. The simulation algorithm [39] computes the match set \( \text{sim}(u) \) for each query node \( u \) via least fixpoint computation. The initial match set \( \text{sim}(u) \) contains all possible candidate matches of \( u \). These match sets are then iteratively refined by removing non-matching nodes. The process stops when a fixpoint is reached.

As shown in Figure 6, the main body of PEval (lines 3-17) is almost identical to the simulation algorithm of [39], except the underlined parts to preprocess fragments. More specifically, PEval first preprocess each fragment \( F_i \) by removing incoming edges and their associated "foreign nodes", and by including nodes to which there exists an outgoing edge from \( F_i \) (lines 1-2). Such preprocessing is conducted to comply with the semantics of simulation relations. More specifically, the match status of a data node \( v \), i.e., whether \( v \) matches some query node \( u \), is determined by the complete match status of all \( v \)'s outgoing neighbors. This also implies that the match status of \( v \) is propagated and updated via the reverse direction of edges linked to \( v \). The preprocessing yields fragment \( F_i \) such that (a) for each node \( v \) in \( V_i \setminus F_i, O \), the outgoing edges from \( v \) are all included in \( E_i \); and (b) for each node \( v' \) in \( F_i, O \), there exists no outgoing edge from \( v' \) present in \( E_i \). As a result, the match status of \( V_i \setminus F_i, O \), i.e., of the nodes owned by \( F_i \), is computed and updated in \( F_i \) at worker \( P_i \); and the match status of nodes in \( F_i, O \) is computed and updated in other fragments.

For each node \( u \in V_Q \), PEval starts with a set \( \text{sim}(u) \) of candidate matches \( v \) in \( F_i \) (lines 3-8), and iteratively removes from \( \text{sim}(u) \) those nodes that violate the simulation condition (lines 9-17). It uses \( \text{post}(v) \) and \( \text{pre}(v) \) to keep track of successors and predecessors of node \( v \), respectively (see [39] for details). It refines \( \text{sim}(u) \) for all \( u \in V_Q \). The partial result \( Q(F_i) \) is designated (line 18).
At the end of the process, PEval sends \( C_i \hat{\bar{x}} = \{x_{u,v} \mid u \in V_Q, v \in F_i.I, x_{u,v} \text{ changed to false} \} \) to coordinator \( P_0 \). That is, the updated match status is propagated via the reverse direction of edges.

At coordinator \( P_0 \), GRAPE maintains \( x_{u,v} \) for all \( u \in \mathcal{F}.I \). Upon receiving messages from all workers, it changes \( x_{u,v} \) to false if it is false in one of the messages. This is specified by \( \text{aggregateMsg} \), taking the order \( \text{false} < \text{true} \). GRAPE identifies those variables that become false, deduces their destinations by referencing \( G_P \), groups them into messages \( M_i \), and sends \( M_i \) to \( P_j \).

(2) IncEval is the sequential incremental simulation algorithm of [28] in response to edge deletions. The changes to \( \text{sim}(u) \) are “equivalent to” removing some nodes from \( \text{sim}(u) \), which can be also seen as the results of removing some relevant edges. Thus propagating the changes of these nodes can be done by propagating the changes of deleted edges. Hence we can use the algorithm of [28] for edge deletions. Note that we just make use of the algorithm for edge deletions as IncEval to process changes to \( x_{u,v} \), but IncEval does not have to handle generic edge deletions in the graph.

As shown in Figure 7, if status variable \( x_{u,v} \) is changed to false by message \( M_i \), it is treated as deleting “cross edges” to \( v \in F_i.O \). Using a stack (line 1), it starts with changed status variables in \( M_i \), propagates the changes to affected area, and removes from sim those matches that become invalid (lines 3-7; see [28] for more details). The partial result is now the revised sim relation (line 8). At the end of the process, IncEval sends to coordinator \( P_0 \) those values of the status variables in \( C_i \hat{\bar{x}} \) that have been set false in the process, along the same lines as how PEval does it.

As shown in [28], IncEval is semi-bounded: its cost is decided by the sizes of “updates” \( |M_i| \) and changes to the affected area necessarily checked by all incremental algorithms for Sim, not by \( |F_i| \). This reduces the cost of iterative computation of graph simulation (the while and for loops).

(3) Assemble simply takes \( Q(G) = \bigcup_{i \in [1, n]} Q(F_i) \), the union of all partial matches, i.e., the sim relation computed at each fragment \( F_i \) at the end of the process.

(4) The correctness of the GRAPE parallelization is warranted by Theorem 4.1, and the monotonic updates to \( C_i \hat{\bar{x}} \). Indeed, \( x_{u,v} \) is initially true for each border node \( v \), and is changed at most once to false, taking the order \( \text{false} < \text{true} \). Furthermore, \( x_{u,v} \) denotes whether \( v \) matches \( u \), as warranted by the correctness of the sequential algorithms [28, 39] (PEval and IncEval).

Subgraph isomorphism. We next parallelize subgraph isomorphism, under which a match of pattern \( Q \) in graph \( G \) is a subgraph of \( G \) that is isomorphic to \( Q \). More specifically, a match of \( Q \) in
Input: $Q = (V_Q, E_Q, L_Q)$, $F_I = (V_I, E_I, L_I)$.
Output: a local annotated version of $N_{d_Q}(s)$ in $F_I$ for each $s \in F_I, I \cup F_I, O'$.

Message preamble:
- an integer variable $\text{dist}(s, t)$ initialized as $\infty$ for each pair $s, t \in V_I$;

1. for each $s \in F_I, I \cup F_I, O'$ do
2. \hspace{1em} $\text{dist}(s, s) := 0; V(s) := \{s\}$;
3. \hspace{1em} queue $\text{Que} := \emptyset; \text{ENQUEUE}(\text{Que}, s)$;
4. while $\text{Que}$ is not empty do
5. \hspace{2em} $u := \text{DEQUEUE}(\text{Que})$;
6. \hspace{2em} if $\text{dist}(s, u) < d_Q$ then
7. \hspace{3em} for each $v$ linked with $u$ do
8. \hspace{4em} if $\text{dist}(s, v) := \infty$ then
9. \hspace{5em} $\text{dist}(s, v) := \text{dist}(s, u) + 1; V(s) := V(s) \cup \{v\}$;
10. \hspace{5em} $\text{ENQUEUE}(\text{Que}, v)$;
11. \hspace{5em} $E(s) := \{(u, v) | (u, v) \in F_I, u, v \in V(s)\}$;
12. \hspace{5em} $L(s) := \{\text{dist}(s, v) | v \in V(s)\}$;
13. $\text{Q}(F_I) := \{(s, V(s), E(s), L(s)) | s \in F_I, I \cup F_I, O'\}$;

Message segment: $M_I := \{(s, V(s), E(s), L(s)) | s \in F_I, I \cup F_I, O'\}$

aggregateMsg = Expand($s$, $V(s)$, $E(s)$, $L(s)$);

Procedure Expand
Input: a source $s \in F_I, I \cup F_I, O'$, $(u, V(u), E(u), L(u))$ for each $u \in \mathcal{F}.I \cup \mathcal{F}.O'$.
Output: the $d_Q$-neighbor $N_{d_Q}(s)$ of $s$ in $G$.

1. queue $\text{Que} := \emptyset; V_Q := V(s)$;
2. for each $v \in V(s)$ do
3. \hspace{1em} if $\text{dist}(s, v) < d_Q$ and $v \in F_I, O \cup F_I, I'$ then
4. \hspace{2em} $\text{ENQUEUE}(\text{Que}, (v, d_Q - \text{dist}(s, v)))$;
5. while $\text{Que}$ is not empty do
6. \hspace{1em} $(u, k) := \text{DEQUEUE}(\text{Que})$;
7. \hspace{1em} use $G_{\text{fr}}$ to find $j$ such that $u \in F_I, I \cup F_J, O'$;
8. \hspace{1em} for each $v \in V(u)$ do
9. \hspace{2em} if $\text{dist}(u, v) \leq k$ then
10. \hspace{3em} $V_Q := V_Q \cup \{v\}$;
11. \hspace{3em} if $v \in F_I, O \cup F_I, I'$ and $\text{dist}(u, v) < k$ then
12. \hspace{4em} $\text{ENQUEUE}(\text{Que}, (v, k - \text{dist}(u, v)))$;
13. $E_Q := \{(u, v) | u, v \in V_Q, (u, v) \in E(w)$ for some $w \in \mathcal{F}.I \cup \mathcal{F}.O'$
14. $N_{d_Q}(s) := (V_Q, E_Q)$;

Fig. 8. PEval for subgraph isomorphism

$G$ is a subgraph $G' = (V', E', L', L'_F)$ of $G$ such that there exists a bijective function $h$ from $V_Q$ to $V'$, where (1) for each node $u \in V_Q$, $L'_F(u) = L'(h(u))$; and (2) $e = (u, u')$ is an edge in $Q$ if and only if $e' = (h(u), h(u'))$ is an edge in $G'$ and $L_Q(e) = L'(e')$.

Graph pattern matching via subgraph isomorphism is to compute the set $Q(G)$ of all matches of $Q$ in $G$. It is intractable: it is NP-complete to decide whether $Q(G)$ is nonempty.

GRAPE parallelizes TurboISO, the sequential algorithm of [37] for subgraph isomorphism. It has two supersteps, one for PEval and the other for IncEval, outlined as follows.

1. PEval identifies update parameters $C_I.x$ at each fragment $F_I$. It declares an integer variable $\text{dist}(s, t)$ as the status variable for each pair of nodes $s$ and $t$ in $F_I$, to record their distance in
Input: Pattern \( Q = (V_Q, E_Q, L_Q) \), fragment \( F_i = (V_i, E_i, L_i) \), message \( M_i \) consisting of \( N_{d_Q}(v) \) for each \( v \in F_i.O \cup F_i.O' \).  
Output: \( Q(F_i \oplus M_i) \), i.e., the set of all matches of \( Q \) in \( F_i \oplus M_i \).

1. \( F_i := F_i \oplus M_i; / * \) extend \( F_i \) with the nodes and edges in \( M_i \) */  
2. \( Q(F_i) := \text{Turbo}_{ISO}(Q, F_i); \)

Fig. 9. IncEval for subgraph isomorphism

fragment \( F_i \). It computes the \( d_Q \)-neighbor \( N_{d_Q}(s) \) of each border node in \( s \in F_i.I \cup F_i.O' \). Here \( d_Q \) is the diameter of pattern \( Q \), i.e., the length of the shortest path between any two nodes in \( Q \) when \( Q \) is treated as an undirected graph; and \( N_d(v) \) is the subgraph of \( G \) induced by the nodes within \( d \) hops of \( v \). At each \( F_i, C_i.x \) consists of \( N_{d_Q}(s) \) for all \( s \in F_i.I \cup F_i.O' \).

Intuitively, upon receiving update parameters \( C_i.x \) from all workers, coordinator \( P_0 \) completes the \( d_Q \)-neighbor of each border node \( s \) in the entire graph \( G \), and sends the \( d_Q \)-neighbor to workers where \( s \) resides, to compensate information loss caused by fragmentation of graph \( G \). After this step, one can directly apply TurboISO to each expanded fragment in parallel.

More specifically, PEval computes \( C_i.x \) at fragment \( F_i \) as shown in Figure 8. PEval performs a standard BFS traversal (Breadth-First Search) from each border node \( s \) in \( F_i.I \cup F_i.O' \) to identify (a) a set \( V(s) \) of nodes that are reachable from \( s \) in \( d_Q \) hops in \( F_i \) (lines 2-10), and (b) a set \( E(s) \) of edges that are associated with nodes in \( V(s) \) (line 11). Here fragment \( F_i \) is treated as an undirected graph in the BFS traversal, ignoring the orientations of the edges (line 7). PEval annotates each node \( v \) in \( V(s) \) with \( \text{dist}(s, t) \) from \( s \) (lines 8-9). These compose a local (annotated) \( d_Q \)-neighbor \( N_{d_Q}(s) \) in fragment \( F_i \). To simplify the discussion, PEval sends these local \( N_{d_Q}(s) \)'s to coordinator \( P_0 \) (line 13). In practice, the union of all these \( d_Q \)-neighbors is sent to \( P_0 \) in a single message. The size of such a message is bounded by the size \( |G| \) of graph \( G \).

Upon receiving the local versions of \( N_{d_Q}(s) \) for all \( s \) in \( F_i.I \cup F_i.O' \), coordinator \( P_0 \) expands each of them to the \( d_Q \)-neighbor \( N_{d_Q}(s) \) in the entire graph \( G \). This is specified by procedure Expand as \text{aggregateMsg}, which performs a BFS-like traversal on the data received and combines necessary nodes and edges, by making use of fragmentation graph \( G_P \) (see Section 2) and the annotations associated with the nodes. A message \( M_i \) is composed and sent to worker \( P_i \) for \( i \in [1, m] \), including all the nodes and edges in the \( d_Q \)-neighbor of \( s \) in the entire graph \( G \), for each \( s \in F_i.O \cup F_i.O' \).

(2) IncEval is the sequential algorithm TurboISO [37]. Given a pattern \( Q \) and a graph \( G \), TurboISO finds all isomorphic matches of \( Q \) in \( G \) as follows. (1) It first picks a start vertex from query \( Q \), and rewrites \( Q \) into a tree \( Q' \) by performing BFS search. Each node in the tree corresponds to a “neighborhood equivalence class” (NEC), by merging nodes with the same labels and neighborhoods. (2) Next, it explores “candidate regions” of \( Q' \), i.e., subgraphs that subsume matches of \( Q \). (3) For each candidate region, it computes an order on the nodes in \( Q' \), based on the number of their candidate matches in the region. (4) It then searches matches within the candidate region in this order. During the search, it only combines partial matches of the NECs, instead of inspecting all possible enumerations. (5) At last, it expands matches of the NECs to get exact matches of \( Q \).

As shown in Figure 9, IncEval computes \( Q(F_i \oplus M_i) \) at each worker \( P_i \) in parallel, on fragment \( F_i \) extended with \( d_Q \)-neighbor of each node in \( F_i.O \cup F_i.O' \) by applying TurboISO. IncEval sends no messages since the values of variables in \( C_i.x \) remain unchanged. As a result, IncEval is executed once, and hence two supersteps suffice.

(3) Assemble simply takes the union of all partial matches computed by IncEval from all workers.
Input: $F_i=(V_i,E_i,L_i)$.
Output: $Q(F_i)$ consisting of $v.cid$ for each $v \in V_i$.

Message preamble: /* candidate set $C_i$ is $F_i.I$ */

- for each $v \in V_i$, an integer variable $v.cid$ initialized as $v$’s id;

1. $CC : = DFS(F_i); /* use DFS to find the set of local CCs */$
2. for each local component $C \in CC$
   3. add a new single root node $v_r$;
   4. $v_r.cid := \min\{v.cid \mid v \in C\}$;
   5. for each node $v \in C$
      6. link $v$ to $v_r$; $v.root := v_r$; $v.cid := v_r.cid$;
   7. $Q(F_i) := \{v.cid \mid v \in V_i\}$;

Message segment: $M_i := \{v.cid \mid v \in F_i.I\}$;
aggregateMsg $= \min(v.cid)$;

Fig. 10. PEval for CC

(4) The correctness of the process is assured by TurboISO and the locality of subgraph isomorphism: a pair $(v, v')$ of nodes in $G$ is in a match of $Q$ only if $v$ is in the $d_Q$-neighbor of $v'$.

5.2 Graph Connectivity

We next study graph connectivity, for computing connected components (CC).

Consider an undirected graph $G$. A subgraph $G_s$ of $G$ is a connected component of $G$ if (a) it is connected, i.e., for any pair $(v, v')$ of nodes in $G_s$, there exists a path between $v$ to $v'$, and (b) it is maximum, i.e., adding any node to $G_s$ makes the induced subgraph no longer connected.

The CC problem is stated as follows, and is known to be in $O(|G|)$ time [13].
- Input: An undirected graph $G=(V, E, L)$.
- Output: All connected components of $G$.

GRAPE parallelizes CC as follows. It picks a sequential CC algorithm as PEval. At each fragment $F_i$, PEval computes its local connected components and creates their ids. The component ids of the border nodes are exchanged with neighboring fragments. The (changed) ids are then used to incrementally update local components in each fragment by IncEval, which simulates a “merging” of two components whenever possible, until no more changes can be made.

(1) PEval declares an integer status variable $v.cid$ for each node $v$ in fragment $F_i$, initialized as its node id. As shown in Figure 10, PEval first uses a standard sequential traversal DFS (Depth-First Search) to compute the local connected components of $F_i$ (line 1). For each local component $C$, (a) PEval creates a “root” node $v_r$ carrying the minimum node id in $C$ as $v_r.cid$ (lines 3-4), and (b) links all the nodes in $C$ to $v_r$, and sets their cid as $v_r.cid$ (lines 5-6). These can be completed in one pass of the edges of $F_i$ via DFS. At the end of process, PEval sends $\{v.cid \mid v \in F_i.I\}$ to coordinator $P_0$. In other words, the set consists of the update parameters at fragment $F_i$.

At $P_0$, GRAPE maintains $v.cid$ for each all $v \in F.I$. It updates $v.cid$ by taking the smallest cid if multiple cids are received, by taking min as aggregateMsg in the message segment of PEval. It groups the nodes with updated cids into messages $M_j$, and sends $M_j$ to $P_j$ by referencing $GP$.

(2) IncEval incrementally updates the cids of the nodes in each fragment $F_i$ upon receiving $M_i$, in parallel, as shown in Figure 11. Observe that message $M_i$ sent to $P_j$ consists of $v.cid$ with updated (smaller) values. For each $v.cid$ in $M_i$, IncEval finds the root $v_r$ of $v$ (line 3), and updates $v_r.cid$
to the minimal one (lines 4-5). IncEval then propagates the changes from every updated root node \( v_r \) to all nodes linked to \( v_r \) by changing their cids to \( v_r.cid \) (lines 6-8). At the end of the process, IncEval sends to coordinator \( P_0 \) the updated cids of nodes in \( F_i.I \) just like in PEval.

One can verify that the incremental algorithm IncEval is bounded: it takes \( O(|M_i|) \) time to identify the root nodes, and \( O(|AFF|) \) time to update cids by following the direct links from the roots, where AFF consists of only those nodes with their cid changed. Hence, it avoids redundant local traversal.

(3) Assemble merges all the nodes having the same cid in a bucket as a single connected component, and returns the set of all these buckets as all the connected components.

(4) Correctness. The process terminates as the cids of the nodes are monotonically decreasing by the definition of aggregateMsg, until no changes can be made. Moreover, it correctly merges two local connected components by propagating the smaller component id.

5.3 Collaborative Filtering

As an example of machine learning, we consider collaborative filtering (CF) [48], a method commonly used for inferring user-product rates in social recommendation. It takes as input a bipartite graph \( G \) that includes two types of nodes, namely, users \( U \) and products \( P \), and a set of weighted edges \( E \subseteq U \times P \). (1) Each user \( u \in U \) (resp. product \( p \in P \)) carries an (unknown) latent factor vector \( u.f \) (resp. \( p.f \)). (2) Each edge \( e = (u, p) \) in \( E \) carries a weight \( r(e) \), estimated as \( u.f^T \ast p.f \) (possibly 0, i.e., “unknown”) that encodes a rating from user \( u \) to product \( p \). The training set \( E_T \) refers to edge set \( \{e \in E \mid r(e) \neq 0\} \), i.e., all the known ratings. The CF problem is as follows.

- Input: Directed bipartite graph \( G \), training set \( E_T \).
- Output: The missing factor vectors \( u.f \) and \( p.f \) that minimizes an error function \( \epsilon(f, E_T) \), estimated as \( \min \sum_{(u,p) \in E_T} (r(u,p) - u.f^T \ast p.f)^2 + \lambda (\|u.f\|^2 + \|p.f\|^2) \).

That is, CF predicts all the unknown ratings by learning the factor vectors that “best fit” \( E_T \).

A common practice to approach CF is to use stochastic gradient descent (SGD) algorithm [48], which iteratively (1) computes a prediction error \( \epsilon(u,p) = r(u,p) - u.f^T \ast p.f \), for each \( e = (u,p) \in E_T \), and (2) updates \( u.f \) and \( p.f \) accordingly towards minimizing \( \epsilon(f, E_T) \).

The SGD algorithm [48] is inherently sequential. To parallelize it, a nice idea has been proposed by DSGD [33], based on a partition of the dataset such that at each round of computation, different workers can process disjoint datasets independently without conflicts. More specifically, it partitions...
**Input:** $F_i = (V_i, E_i, L_i)$.

**Output:** $Q(F_i)$ consisting of $v.f$ for each $v \in V_i$.

**Message preamble:** /* candidate set $C_i$ is $F_i.I$ */

- a variable $x.v = (v.f, t)$ for each $v \in V_i$;

1. $B_i := \{ e \in E(i, i) \mid r(e) \neq \emptyset \}$;
2. Run SGD on the training set $B_i$;
3. $t := t + 1$;
4. $Q(F_i) := \{ (v.f \mid v \in V_i) \}$;

**Message segment:** $M_t := \{ (v.f, t) \mid v \in F_i.I, v.f$ changed $\}$

**Procedure** SGD

**Input:** A training set $B$.

**Output:** Revised training set.

/* SGD on the training set $B$ (pseudo-code)*/

1. **for each** $k \in \{1, 2, \ldots, |B|\}$ **do**
2. \hspace{1em} Pick an edge $(u, p)$ from $B$ uniformly at random;
3. \hspace{1em} $\epsilon(u, p) := r(u, p) - u.f^T \ast p.f$;
4. \hspace{1em} $u.f^t := u.f + \gamma(\epsilon(u, p) \ast p.f - \lambda \ast u.f)$;
5. \hspace{1em} $p.f := p.f + \gamma(\epsilon(u, p) \ast u.f - \lambda \ast p.f)$;
6. \hspace{1em} $u.f := u.f^t$;

---

**Fig. 12.** PEval for CF

the user set $U$ into $m$ disjoint subsets $U(1), U(2), \ldots, U(m)$, and similarly, the product set $P$ into disjoint $P(1), P(2), \ldots, P(m)$ such that $U = \bigcup_{i=1}^{m} U(i)$ and $P = \bigcup_{j=1}^{m} P(j)$, for a constant $m$. Correspondingly the training set $E$ is divided into $m^2$ blocks, such that each $1 \leq i, j \leq m$, a block $E(i, j)$ identified by a pair $(i, j)$ is the subset of $E$ induced by $U(i)$ and $P(j)$. Clearly $E = \bigcup_{1 \leq i, j \leq m} E(i, j)$. Two blocks $E(i, j)$ and $E(i', j')$ are independent if $i \neq i'$ and $j \neq j'$. DSGD parallelizes SGD by utilizing the property that the factor vectors of independent blocks can be updated in parallel without conflicts.

Adopting the partition strategy of DSGD, GRAPE parallelizes the sequential SGD algorithm such that different workers can run SGD on different fragments of a graph $G$ in parallel, without conflicts. GRAPE partitions $G$ by a vertex-cut strategy and distributes the $m^2$ blocks into $m$ different fragments. More specifically, it defines $F_i = (V_i, E_i, L_i)$, where $V_i = U(i) \cup \bigcup_{j=1}^{m} P(j)$ and $E_i = \bigcup_{j=1}^{m} E(i, j)$, i.e., $P$ is shared by all fragments while $U$ is partitioned across different workers.

(1) PEval declares a status variable $v.x = (v.f, t)$ for each node $v$, where $v.f$ is the factor vector of $v$ (initially $\emptyset$), and $t$ is an integer (initially 0) that bookkeeps a timestamp at which $v.f$ is lastly updated. The candidate set $C_i$ the border nodes set $F_i.I$.

As shown in Figure 12, PEval essentially runs the sequential SGD algorithm of [48] on the training block $E(i, i)$ as follows. Each time it picks an edge $(u, p)$ from the training set uniformly at random and computes the prediction error $\epsilon(u, p)$. It updates local factor vectors by a magnitude proportional to $\gamma$ in the opposite direction of the gradient as:

$$u.f^t = u.f^{t-1} + \gamma(\epsilon(u, p) \ast p.f^{t-1} - \lambda \ast u.f^{t-1})$$  \hspace{1em} (1)

$$p.f^t = p.f^{t-1} + \gamma(\epsilon(u, p) \ast u.f^{t-1} - \lambda \ast p.f^{t-1})$$  \hspace{1em} (2)
Input: $F_i = (V_i, E_i, L_i)$, partial result $Q(F_i)$,
message $M_i$ including updated factor vectors and
a pair $(i, p_i)$ indicates the training block.
Output: $Q(F_i \oplus M_i)$.

1. for each $v^{\text{in}}, f \in M_i$ do
2. \hspace{1em} $v.f := v^{\text{in}}, f$;
3. $B_i := \{ e \in E(i, p_i) \mid r(e) \neq 0 \}$;
4. Run SGD on the training set $B_i$;
5. $t := t + 1$;
6. $Q(F_i) := \{ v.f \mid v \in V_i \}$;

Message segment:
$M_i := \{ (v.f, t) \mid v \in F_i.I, v.f \text{ changed } \}$;

Fig. 13. IncEval for CF

By the partition strategy, the training blocks $E(1, 1), E(2, 2), \ldots, E(d, d)$ on different fragments line on the diagonal of the rating matrix, and are independent of each other. At the end of its process, 
PEval sends message $M_i$ that consists of updated $v.x$ for nodes $v \in C_i$ to coordinator $P_0$.

At coordinator $P_0$, GRAPE maintains $v.x = (v.f, t)$ for all border nodes $v \in F.I = F.O$. Upon receiving updated values $(v.f', t')$ with $t' > t$, it changes $v.f$ to $v.f'$, i.e., it defines aggregateMsg as $\text{max}$ on timestamps. This is well defined since different workers process independent blocks.

GRAPE then groups the updated vectors into messages $M_j$, and sends $M_j$ to $P_j$ as usual. That is, GRAPE passes the latest updates to factor vectors to workers.

In addition, coordinator $P_0$ selects $m$ independent blocks to be processed in the next round. To do this $P_0$ simply picks a permutation $p_1, p_2, \ldots, p_m$ of $\{1, 2, \ldots, m\}$ following some fixed strategy, e.g., simple cycle scheduling. It sends a pair $(j, p_j)$ along with $M_j$ to $P_j$. By the partition strategy, block $E(j, p_j)$ belongs to $F_j$ and $E(j, p_j)$ is independent of $E(i, p_i)$ if $j \neq i$.

(2) IncEval iteratively updates the factor vectors of independent blocks. As shown in Figure 13, IncEval first updates the factor vectors with the latest changes (lines 1-2). It then extracts the training set $B_i$ for the current round based on the block identifier assigned by $P_0$ (line 3), and runs the sequential SGD algorithm [48] on $B_i$ just like PEval (line 4). Since the training sets $B_1, B_2, \ldots, B_d$ are extracted from the independent blocks $E(1, p_1), E(2, p_2), \ldots, E(d, p_d)$, they can be processed in parallel without conflict. At the end of the process, it sends the updated vectors in $C_i$ like PEval.

(3) Assemble simply takes the union of all the factor vectors of nodes from all the workers.

(4) Correctness. Observe that a permutation $p_1, p_2, \ldots, p_m$ of $\{1, 2, \ldots, m\}$ corresponds to a $m$-monomial stratum of DSGD [33]. The permutation in each round is picked according to a stratum selection strategy. It is known that the strategy guarantees the convergence of DSGD (see [33] for more details). As a result, GRAPE converges and correctly infers CF models by the correctness of DSGD.

6 IMPLEMENTATION OF GRAPE
We next outline an implementation of parallel graph engine GRAPE.

Architecture overview. GRAPE adopts a four-tier architecture depicted in Figure 14.

(1) Its top layer is a user interface. As shown in Figure 1, GRAPE supports interactions with (a) developers who specify and register sequential PEval, IncEval and Assemble as a PIE program for
a class \( Q \) of graph queries (the plug panel); and (b) end users who make use of PIE programs from API library, pick a graph \( G \), enter queries \( Q \in Q \), and “play” (the play panel). GRAPE parallelizes the PIE program, computes \( Q(G) \) and displays \( Q(G) \) in result and analytics consoles.

(2) At the core of the system is a parallel query engine. It manages sequential algorithms registered in GRAPE API, makes parallel evaluation plans for PIE programs, and executes the plans for query answering (see Section 3.1). It also enforces consistency control and fault tolerance (see below).

(3) Underlying the query engine are (a) an MPI Controller (message passing interface) for communications between coordinator and workers, (b) an Index Manager for loading indices, (c) a Partition Manager to partition graphs, and (d) a Load Balancer to balance workload (see below).

(4) The storage layer manages graph data in DFS (distributed file system). It is accessible to the query engine, Index Manager, Partition Manager and Load Balancer.

**Message passing.** The MPI Controller of GRAPE makes use of a standard MPI for parallel and distributed programs. It currently adopts MPICH [5], which is also the basis of other parallel graph systems such as GraphLab [49] and Blogel [71]. It generates messages and coordinates messages in synchronization steps using standard MPI primitives.

We remark that at the conceptual level, to simplify the discussion, we adopt a coordinator to aggregate messages (Section 3). In practice, GRAPE implements point-to-point message passing instead: workers exchange messages directly without going through a coordinator, accumulate messages received in a buffer, and the aggregation function is invoked at each worker. It is easy to verify that this implementation and the centralized aggregation with coordinator produce the same results, since the aggregation function is invoked after all messages are received.

**Graph partition.** The Graph Partitioner supports a variety of built-in partition algorithms. Users may pick (a) METIS, a fast heuristic algorithm for sparse graphs [44], (b) edge-cut partition [12, 18] and vertex-cut partition [47], (c) 1-D and 2-D partitions [17], which distribute vertex and adjacent matrix to the workers, respectively, emphasizing on maximizing the parallelism of graph traversal, and (d) a fast streaming-style partition strategy [62] that assigns edges to high degree nodes to reduce cross edges. New data partition strategies can also be deployed at GRAPE.

**Multi-thread.** GRAPE supports multi-threading. At each worker, there are multiple working threads, each acting as a virtual worker and handling one fragment. During computation, the threads at the same worker are maintained in a pool; a main thread at the worker takes the responsibility
of assigning fragments and workload to idle threads in the pool. At the end of each round of the computation, the main thread generates messages and communicates with peer workers. The main thread is able to process messages in a buffer even when its working threads are still computing. This allows workers to overlap computation and communication, and reduce response time.

Graph-level optimization. In contrast to prior graph systems, GRAPE supports data-partitioned parallelism by parallelizing the runs of sequential algorithms. Since fragments of a graph are graphs themselves, all optimization strategies developed for sequential (batch and incremental) algorithms can be readily used by GRAPE, to improve the performance of PEval and IncEval over graph fragments. As examples, below we outline some of the graph-level optimization strategies.

(1) Indexing. Any indexing structure effective for sequential algorithm can be computed offline and directly used to optimize PEval, IncEval and Assemble. GRAPE can support indices including (1) 2-hop index [21] for reachability queries; and (2) neighborhood-index [45] for candidate filtering in graph pattern matching. Moreover, new indices can be incorporated into GRAPE API library.

(2) Compression. Another strategy is query preserving compression [26] at the fragment level. Given a query class \( Q \) and a fragment \( F_i \), each worker \( P_i \) computes a smaller \( F^c_i \) offline via a compression algorithm, such that for any query \( Q \) in \( Q \), \( Q(F_i) \) can be computed from \( F^c_i \) without decompressing \( F^c_i \), regardless of what sequential PEval and IncEval are used. As shown in [26], this compression scheme is effective for graph pattern matching and graph traversal, among other things.

(3) Dynamic grouping. GRAPE dynamically groups a set of border nodes by adding a “dummy” node, and sends messages from the dummy nodes in batches, instead of one by one. This effectively reduces the amount of message passing in each synchronization step.

To the best of our knowledge, many of these optimization strategies are not supported by the state-of-the-art vertex-centric and block-centric graph query systems. For instance, indexing and query-preserving compression for sequential algorithms do not carry over to vertex-centric programs, and block-centric programming essentially treats blocks as vertices rather than graphs.

Fault tolerance. GRAPE employs an arbitrator mechanism to recover from both worker failures and coordinator failures (a.k.a. single-point failures). More specifically, it reserves a worker \( P_a \) as arbitrator, and a worker \( S_c' \) as a standby coordinator. It keeps sending heart-beat signals to all workers and the coordinator. In case of failure, (a) if a worker fails to respond, the arbitrator transfers its computation tasks to another worker; and (b) if the coordinator fails, it activates the standby coordinator \( S_c' \) to continue parallel computation. It is also possible for GRAPE to adopt the optimistic recovery mechanism introduced in [60] for general fixpoint paradigm [15].

Consistency. Multiple workers may update copies of the same status variable. To cope with this, (a) GRAPE allows users to specify a conflict resolution policy as function \texttt{aggregateMsg} in PEval (Section 3.2), e.g., \texttt{min} for SSSP and CC (Section 5), based on a partial order on the domain of status variables, e.g., linear order on integers. Based on the policy, inconsistencies are resolved in each synchronization step of PEval and IncEval processes. Moreover, Theorem 4.1 guarantees the consistency when the policy satisfies the monotonic condition. (b) GRAPE also supports default exception handlers when users opt not to specify \texttt{aggregateMsg}. In addition, GRAPE allows users to specify generic consistency control strategies and register them in GRAPE API library.

7 EXPERIMENTAL STUDY

Using real-life and synthetic graphs, we next empirically evaluate GRAPE, for its (1) efficiency and scalability, (2) communication costs, (3) effectiveness of incremental steps, and (4) compatibility
with optimization techniques developed for sequential graph algorithms. We used real-life graphs larger than those that [31] experimented with. We evaluated the performance of GRAPE compared with Giraph (a open-source version of Pregel), GraphLab, and Blogel (the fastest block-centric system we are aware of). We compared GRAPE with the prior graph systems by parallelizing existing sequential algorithms with a preliminary implementation of GRAPE [9].

**Experimental setting.** We used five real-life graphs of different types, including

1. movieLens [3], a dense recommendation network (bipartite graph) that has 20 million movie ratings (as weighted edges) between 138000 users and 27000 movies;
2. UKWeb [1], a Web graph with 133 million nodes and 5 billion edges;
3. DBpedia [7], a knowledge base with 5 million entities and 54 million edges, with 411 labels;
4. Friendster [4], a social network with 65 million users and 1.8 billion links; and
5. traffic [2], a road network with 23 million nodes (locations) and 58 million edges.

To make use of unlabeled Friendster for Sim and SubIso, we assigned up to 100 random labels to nodes. We also randomly assigned weights to UKWeb, traffic and Friendster for testing SSSP.

**Synthetic graphs.** To evaluate the scalability of GRAPE (Exp-1 and Exp-2), we also developed a generator to produce synthetic graphs \( G = (V, E, L) \) controlled by the numbers of nodes \( |V| \) (up to 250 million) and edges \( |E| \) (up to 2.5 billion), with \( L \) drawn from an alphabet \( \mathcal{L} \) of 100 labels.

**Partitioning and Loading.** We used XtraPuLP [61] as the default graph partition strategy. In theory, GRAPE works regardless of what partitioning strategy is used, and guarantees to converge under the conditions given in Theorem 4.1. In practice, different strategies may yield partitions with various degrees of skewness and stragglers, which have an impact on the performance of GRAPE. Here we picked XtraPuLP, which is widely used in practice. On Friendster, for example, XtraPuLP took about 16 minutes, and our computations took at most 62 seconds. However, graph partitioning is performed once offline. Afterwards various queries are answered online on the same partition. The partitioning costs for traffic, UKWeb, DBpedia and movieLens are 6.0, 598.1, 32.2, 4.3 seconds, respectively.

GRAPE loads graph data from a distributed file system by each worker simultaneously. It takes about 20 minutes to import Friendster by 4 workers at the first time (16s, 24m, 44s, 10s for traffic, UKWeb, DBpedia, movieLens, respectively). After the first loading, the graph is “serialized” to the storage in a compact format, which largely reduces the loading time to 40s (2s, 86s, 4s, 2s for traffic, UKWeb, DBpedia, movieLens, respectively) for reloading afterwards when necessary.

It should be remarked that GRAPE is able to load a graph \( G \) once and process query workload (i.e., a set of queries) posed on \( G \), without reloading \( G \). In contrast, GraphLab, Giraph and Blogel require the graph to be reloaded each time a single query is issued, and loading is costly over large graphs. In favor of these systems, we exclude the loading cost when reporting the experimental results.

**Queries.** We randomly generated the following queries for SSSP, Sim and SubIso. (a) We sampled 10 source nodes in each graph used, and constructed an SSSP query for each node. (b) We generated 20 pattern queries for Sim and SubIso, controlled by \( |Q| = (|V_Q|, |E_Q|) \), the number of nodes and edges, respectively, using labels drawn from the graphs experimented with.

**Algorithms.** We implemented the PIE programs (PEval, IncEval and Assemble) for the query classes given in Sections 3 and 5, namely, SSSP, Sim, SubIso, CC and CF, which are registered in the API library of GRAPE. We adopted basic sequential algorithms, and only used optimized Sim to demonstrate how GRAPE inherits optimization strategies developed for sequential algorithms (Exp-3).

We also implemented algorithms for these query classes for Giraph, GraphLab and Blogel. We used the “default” code provided by the systems when available, and made our best efforts to
develop “optimal” algorithms otherwise. We also used the “default” graph partition algorithms provided by these systems, i.e., hash partitioning for GraphLab and Giraph, and Voronoi partitioning for Blogel. We implemented synchronized algorithms for both GraphLab and Giraph for the ease of comparison. As observed by [40, 41, 68], neither asynchronous model nor synchronous model outperform the other for different algorithms, input graphs and cluster scales. We expect the observed relative performance trends to hold on other similar graph systems.

We deployed the systems on a cluster of up to 12 machines, each with 16 processors (Intel Xeon 2.2GHz) and 128G memory (thus in total 192 processors). This is the best configuration we could afford. Each experiment was repeated 5 times and the average is reported here.

**Experimental results.** We next report our findings.

**Exp-1: Efficiency.** We first evaluated the efficiency and scalability of GRAPE by varying the number \( n \) of processors used, from 64 to 192. For each algorithm, we chose datasets based on its applications in the real world, to demonstrate meaningful computations. For SSSP and CC, we experimented with real-life graphs UKWeb, traffic and Friendster. For Sim and SubIso, we used Friendster and DBPedia. We used MovieLens for CF as its application in movie recommendation.

1) SSSP. Figures 15a-15c report the performance of the systems for SSSP over Friendster, UKWeb and traffic, respectively. We report the average over 10 SSSP queries on each graph. The results on other graphs are consistent (not shown). From the results we can see the following.

(a) GRAPE outperforms Giraph, GraphLab and Blogel by 14842, 3992 and 756 times, respectively, over traffic with 192 processors (Figure 15a). In the same setting, it is 556, 102 and 36 times faster over UKWeb (Figure 15b), and 18, 1.7 and 4.6 times faster over Friendster (Figure 15c). These results demonstrate that by simply parallelizing sequential algorithms without further optimization, GRAPE already outperforms the state-of-the-art systems in response time for SSSP.

The improvement of GRAPE over all the systems on traffic is much larger than on Friendster and UKWeb since the traffic graph has a larger diameter. In addition, (i) for Giraph and GraphLab, this is because synchronous vertex-centric algorithms take more supersteps to converge on graphs with large diameters, such as traffic. Using 192 processors, Giraph take 10749 supersteps over traffic and 161 over UKWeb; similarly for GraphLab. In contrast, GRAPE is not vertex-centric and it takes 31 supersteps on traffic and 24 on UKWeb. (ii) Blogel also takes more (1690) supersteps over traffic than over UKWeb (42 supersteps) and Friendster (23 supersteps). It generates more blocks over traffic (with larger diameter) than UKWeb and Friendster. Since Blogel treats blocks as vertices, the benefit of parallelism is degraded with more blocks.

(b) In all cases, GRAPE take less time when \( n \) increases. On average, it is 1.4, 2.3 and 1.5 times faster for \( n \) from 64 to 192 over traffic, UKWeb and Friendster, respectively. (i) Compared with the results in [31] using less processors, this improvement degrades a bit. This is mainly because the larger number of fragments leads to more communication overhead. On the other hand, such impact is significantly mitigated by IncEval that only ships changed update parameters. (ii) In contrast, Blogel does not demonstrate such consistency in scalability. It takes more time on traffic when \( n \) is larger. When \( n \) varies from 160 to 192, it also takes longer over Friendster. Its communication cost dominates the parallel cost as \( n \) grows, “canceling out” the benefit of parallelism. (iii) GRAPE has scalability comparable to GraphLab over Friendster and scales better over UKWeb and traffic. Giraph has better improvement with larger \( n \), but with constantly higher cost (see (a)) than GRAPE.

(c) GRAPE significantly reduces supersteps. It takes on average 22 supersteps, while Giraph, GraphLab and Blogel take 3647, 3647 and 585 supersteps, respectively. This is because GRAPE runs sequential algorithms over fragmented graphs with cross-fragment communication only
when necessary, and moreover, IncEval ships only changes to status variables. In contrast, Giraph, GraphLab and Blogel pass vertex-vertex (vertex-block) messages.

(d) SSSP under Blogel runs in VB-model. In each superstep, it first runs V-compute over all vertices to identify “active” vertices, i.e., vertices whose distance value is updated; it then runs B-compute on active vertices within blocks. Compared with pure vertex-centric models, running a sequential algorithm within blocks reduces communication cost. However, its V-compute incurs redundant computations since it runs over all vertices in each superstep. In contrast, GRAPE runs sequential algorithms within partitions and leverages incremental computation to reduce redundant computation and communication cost. In each round, IncEval only runs on affected vertices.
(2) CC. Figures 15d-15e report the performance for CC detection, and tell us the following. (a) Both GRAPE and Blogel substantially outperform Giraph and GraphLab. For instance, when \( n = 192 \), GRAPE is on average 12094 and 1329 times faster than Giraph and GraphLab, respectively. (b) Blogel is faster than GRAPE in some cases, e.g., 3.5 seconds vs. 17.9 seconds over Friendster when \( n = 192 \). This is because Blogel embeds the computation of CC in its graph partition phase as precomputation, while this graph partition cost (on average 357 seconds using its built-in Voronoi partition) is not included in its response time. In other words, without precomputation, the performance of GRAPE is already comparable to the near “optimal” case reported by Blogel.

CC in GRAPE also works better than the one in Giraph++ [63]. This is because after exchanging messages between blocks, Giraph++ invokes computation on all internal vertices, and a large part of the computation is redundant. In contrast, IncEval of GRAPE processes only those affected vertices, by capitalizing on auxiliary indices that were inherited from sequential algorithms.

(3) Sim. Fixing \( |Q| = (6, 10) \), i.e., patterns \( Q \) with 6 nodes and 10 edges, we evaluated graph simulation over DBpedia and Friendster. As shown in Figures 15g-15h, (a) GRAPE consistently outperforms Giraph, GraphLab and Blogel over all queries. It is 109, 8.3 and 45.2 times faster over Friendster, and 136.7, 5.8 and 20.8 times faster over DBpedia for 20 queries on average, respectively, when \( n = 192 \). (b) GRAPE scales better with the number \( n \) of processors than the others. (c) GRAPE takes at most 21 supersteps, while Giraph, GraphLab and Blogel take 38, 38 and 40 supersteps, respectively. This empirically validates the convergence guarantee of GRAPE under monotonic status variable updates and its effect on reducing computation and communication costs.

(4) Subso. Fixing \( |Q| = (3, 5) \), we evaluated the performance of the systems for subgraph isomorphism. As shown in Figures 15i-15j over Friendster and DBpedia, respectively, (a) GRAPE is on average 76, 35 and 9 times faster than Giraph, GraphLab and Blogel when \( n = 192 \). (b) When \( n \) varies from 64 to 192, GRAPE is on average 1.3 and 1.2 times faster over Friendster and DBpedia, respectively. This is comparable with GraphLab that is 1.3 and 2.8 times faster, respectively.

(5) CF. For collaborative filtering, we used real-life movieLens [3] with a training set \( |E_T| = 90\%|E| \). We compared GRAPE with the built-in SGD-based CF in GraphLab, and with CF implemented for Giraph and Blogel. It should be remarked that CF favors “vertex-centric” programming since each user or product node only needs to exchange data with its neighbors, as indicated by that GraphLab and Giraph outperform Blogel. Nonetheless, as shown in Figure 15k, GRAPE is on average 4.1, 2.6 and 12.4 times faster than Giraph, GraphLab and Blogel, respectively, when the number of processors varies from 64 to 192. Moreover, GRAPE scales well with \( n \).

(6) Scalability of GRAPE. As observed in [51], the speed-up of a system may degrade over more processors. We thus evaluated the scalability of GRAPE, which measures the ability to keep the same performance when both the size of graph \( G \) (denoted as \(|V|, |E|\)) and the number \( n \) of processors increase proportionally. We varied \( n \) from 64 to 192, and for each \( n \), deployed GRAPE over a synthetic graph. The graph size varies from \((50M, 500M)\) (i.e., 50 million nodes and 500 million edges; denoted as \( G_1 \)) to \((250M, 2.5B)\) (denoted as \( G_5 \)), with fixed ratio between edge number and node number and proportional to \( n \). The scalability at e.g., \((128, G_3)\) is the ratio of the time using 64 processors over \( G_1 \) to its counterpart using 128 processors over \( G_3 \). As shown in Fig. 15l, GRAPE preserves a reasonable scalability (close to linear scalability, the optimal scalability).

We further evaluated the COST [51] of GRAPE, which denotes the hardware configuration (the number of cores) required by GRAPE to outperform a competent single-threaded implementation. It measures the extra overhead (e.g., communication) introduced by parallel systems relative to single-threaded implementations. The results are reported in Table 3. For CC, we adopted its
original implementation\(^1\) of [51] as the single-threaded version. For SSSP, Sim, SubIso and CF, no implementations are given in [51], and we adopted the best single-threaded implementations to our knowledge for comparison with GRAPE. Following [51], for large input graphs that are unable to fit into RAM, we used the external I/O on SSD as an extension to RAM (marked with * in Table 3).

From Table 3 we can see the following. (1) For SSSP, CC, Sim and CF, GRAPE achieves speed-up over single-threaded implementations with just 2 or 4 cores over all tested input graphs. (2) For SubIso, even with its relatively heavy prefetching cost (Section 5.1), GRAPE still outperforms the single-threaded implementations with 24 or 32 cores (just 2 physical machines). (3) According to [51], GraphLab had a COST of 512 cores and Spark GraphX had unbounded COST (no configuration can outperform single-threaded). Therefore, GRAPE demonstrates better scalability than GraphLab and GraphX, with smaller extra overhead for parallel graph computations.

It should be remarked that parallelization overheads are inevitable for all distributed/parallel systems, including but not limited to GRAPE. Nonetheless, parallel processing often works better when dealing with large-scale graphs that are beyond the capacity of a single machine.

**Exp-2: Communication cost.** The communication cost (in bytes) reported by Giraph, GraphLab and Blogel depends on their own implementation of message blocks and protocols. As observed in [36], these built-in message or byte counters differ from each other: Blogel counts cross-process bytes, GraphLab reports cross-machine bytes, and Giraph tracks cross-partition bytes. For a fair comparison, we adopted a third-party tool Nethogs [10] following the practice [36]. It tracks the total bytes sent by each machine during the run, by monitoring the system file /proc/net/dev. This metric, better aligned to parallel models of the systems, reveals consistent results with better insights.

In the same setting as Exp-1, Figure 16 reports the communication costs of the systems. The results show that in all cases, GRAPE incurs much less communication cost than Giraph and GraphLab. On datasets excluding traffic, with 192 processors, it ships on average 0.08%, 1.1%, 0.3%, 0.18% and 8.4% of the data shipped for SSSP, Sim, CC, SubIso and CF by Giraph, and 0.11%, 0.14%, 0.3%, 0.19% and 44% by GraphLab, respectively; moreover, it reduces their cost by 6 and 5 orders of magnitude for SSSP and CC on traffic, respectively. While it ships more data than Blogel for CC due to the precomputation of Blogel remarked earlier, it only ships 6.2%, 0.1%, 1.9% and 4.8% of the data shipped by Blogel for Sim, SubIso, SSSP and CF, respectively. On traffic, GRAPE also reduces the communication cost of Blogel by 4 and 3 orders of magnitude for SSSP and CC, respectively.

\(^1\)https://github.com/frankmcsherry/COST

| Algorithms | Dataset | GRAPE cores | GRAPE time (s) | Single-threaded time (s) |
|------------|---------|-------------|----------------|--------------------------|
| SSSP       | traffic | 4           | 6.08           | 6.14                     |
|            | Friendster | 4         | 96.3           | 101.1                    |
|            | UKWeb    | 2           | 149.1          | 151.8*                   |
| CC         | traffic | 2           | 1.52           | 1.63                     |
|            | Friendster | 4         | 35.5           | 40.3                     |
|            | UKWeb    | 2           | 21.6           | 27.9*                    |
| Sim        | DBpedia | 2           | 7.11           | 7.32                     |
|            | Friendster | 2         | 44.0           | 93.7*                    |
| SubIso     | DBpedia | 24          | 0.08           | 0.08                     |
|            | Friendster | 32        | 20.4           | 25.0*                    |
| CF         | movieLens | 2         | 460.0          | 733                      |

Table 3. COST of GRAPE
Fig. 16. Communication costs

(1) SSSP. Figures 16a-16c show that both GRAPE and Blogel incur communication costs that are orders of magnitudes less than those of GraphLab and Giraph. This is because vertex-centric programming incurs a large amount of messages. Both block-centric programs (Blogel) and PIE programs (GRAPE) reduce unnecessary messages, and trigger inter-block communication only when necessary. We also observe that GRAPE ships 0.9% and 10% of the data shipped by Blogel over UKWeb and Friendster, respectively. Indeed, GRAPE ships only changed values of update parameters, and needs fewer supersteps. These significantly reduce the size and number of messages.

(2) CC. Figures 16d-16f demonstrate similar improvement of GRAPE over GraphLab and Giraph for CC. It ships on average 0.2% and 0.3% of the data shipped by Giraph and GraphLab on datasets excluding traffic, and 0.0015% and 0.0003% on traffic, respectively. Since Blogel precomputes CC
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Fig. 17. Incremental steps and optimization

(a) The impact of IncEval

(b) Optimization on GRAPE

(see Exp-1(2)), it ships little data. Nonetheless, GRAPE is not far worse than the near “optimal” case of Blogel on Friendster and UKWeb, and ships only 0.05% of the data shipped by Blogel on traffic.

(3) Sim. Figures 16g and 16h report the communication cost for graph simulation over Friendster and DBpedia, respectively. One can see that GRAPE ships substantially less data, e.g., on average 0.9%, 0.1%, 4.9% of the data shipped by Giraph, GraphLab and Blogel, respectively. Observe that the communication cost of Blogel is much higher than that of GRAPE, even though it adopts inter-block communication. This shows that the extension of vertex-centric to block-centric by Blogel may not suffice to reduce messages when it comes to complex queries. GRAPE works better than these systems by employing incremental IncEval to reduce redundant messages and computation.

(4) SubIso. Figures 16i and 16j report the results for SubIso over Friendster and DBpedia, respectively. The results are consistent with their counterparts for Sim. On average, GRAPE ships 0.18%, 0.24% and 3.2% of the data shipped by Giraph, GraphLab and Blogel, respectively.

(5) CF. Figure 16k reports the result for CF over movieLens. On average, GRAPE ships 5.6%, 43.3% and 3.2% of the data shipped by Giraph, GraphLab and Blogel, respectively.

(6) Synthetic. In the same setting as Figure 15l, Figure 16l reports the communication cost for SSSP using synthetic graphs. The results demonstrate that more communication cost is incurred over larger graphs and more processors, due to increased border nodes, as expected.

Exp-3: Incremental computation. We evaluated the effectiveness of incremental IncEval. We implemented a batch version of GRAPE for Sim queries, denoted as GRAPE\textsubscript{NI}, which uses PEval to perform iterative computations and handle the messages, instead of IncEval. It mimics the case when no incremental computation is used. As shown in Figure 17a over Friendster, (1) GRAPE outperforms GRAPE\textsubscript{NI} by 9.0 times with 192 processors; and (2) the gap is larger when less processors are employed, e.g., 11.0 times when 64 processors are used. This is because the less processors are used, the larger fragments reside at each processor, and as a consequence, heavier computation costs are incurred at each superstep. This verifies that incremental steps effectively reduces redundant local computations in iterative graph computations. The results on DBpedia are consistent (not shown).

Exp-4. Compatibility. We also evaluated the compatibility of optimization strategies developed for sequential graph algorithms with GRAPE parallelization. For a query class $Q$, a sequential algorithm $\mathcal{A}$ and its optimized version $\mathcal{A}^*$ for $Q$, denote the speedup of the optimization as $\frac{T(\mathcal{A})}{T(\mathcal{A}^*)}$. Denote the running time of GRAPE parallelization of $\mathcal{A}$ (resp. $\mathcal{A}^*$) as $T_p(\mathcal{A})$ (resp. $T_p(\mathcal{A}^*)$) for a given number $n$ of processors. Ideally, $\frac{T(\mathcal{A})}{T(\mathcal{A}^*)}$ should be close to $\frac{T_p(\mathcal{A})}{T_p(\mathcal{A}^*)}$, i.e., GRAPE preserves the speedup from the optimization. That is, the impact of the optimization is not “dampened out” by parallelization overhead such as synchronization and message passing.
We make a case for graph simulation. We evaluated two sequential algorithms, one from [39], and the other is an optimized version that employs indices to reduce candidates [25]. Using Sim queries over Friendster, we found that the average speedup of sequential algorithms is 1.24. Varying \( n \) from 64 to 192, we report the speedup of the parallelized algorithms of GRAPE in Figure 17b. The results on DBpedia are consistent (not shown). The results suggest that the speedup is close to its sequential counterpart. Such optimization cannot be easily encoded in vertex programs of Giraph and GraphLab and the V-mode and B-mode programs of Blogel.

Summary. From the experimental results we find the following:

1. By simply parallelizing sequential algorithms, the performance of GRAPE is already comparable to state-of-the-art systems. Using from 64 to 192 processors over real-life graphs excluding traffic, GRAPE is on average 484, 36 and 15 times faster than Giraph, GraphLab and Blogel for SSSP, 151, 6.8 and 16 times for Sim, 149.3, 34.2 and 9.6 times for SubIso, and 4.6, 2.6 and 12.4 for CF, respectively. For CC, it is 1377 and 212 times faster than Giraph and GraphLab, respectively, and is comparable to the “optimal” case of Blogel although Blogel embeds the computation of CC in its graph partition phase. On traffic, for SSSP and CC, GRAPE is on average 4, 3 and 2 orders of magnitude faster than Giraph, GraphLab and Blogel, respectively. The results on synthetic graphs are consistent.

2. In the same setting, on datasets excluding traffic GRAPE ships on average 0.07%, 0.12% and 1.7% of the data shipped across machines by Giraph, GraphLab and Blogel for SSSP, 0.89%, 0.14% and 4.9% for Sim, 0.18%, 0.23% and 0.11% for SubIso, 5.6%, 43.3% and 3.2% for CF, respectively. For CC, it incurs 0.23% and 0.3% of data shipment of Giraph and GraphLab, and is comparable with “optimized” Blogel. On traffic, for SSSP and CC, it ships on average 5, 6 and 3 orders of magnitude less data shipment by Giraph, GraphLab and Blogel, respectively.

3. GRAPE demonstrates good scalability when using more processors, since its incremental computation mitigates the impact of more border nodes and fragments.

4. Incremental steps effectively reduce iterative recomputation. For Sim, it improves the response time by 9.6 times on average.

5. GRAPE inherits the benefit of optimized sequential algorithms. For Sim, it is on average 20% faster by using the algorithm of [25] instead of the algorithm of [39].

8 CONCLUSION

We have proposed an approach to parallelizing sequential graph algorithms. Given a class \( Q \) of graph queries, users can devise existing sequential algorithms for \( Q \) with minor changes, without recasting the entire algorithms into a new model. GRAPE parallelizes the computation and guarantees to converge at correct answers under a monotonic condition, as long as the sequential algorithms are correct. Moreover, graph algorithms that are developed for existing parallel graph systems can be migrated to GRAPE, without incurring extra complexity. We have verified that GRAPE achieves comparable performance to the state-of-the-art graph systems for various query classes, and that (bounded) IncEval effectively reduces unnecessary recomputation and hence the cost of iterative graph computations. We hope that GRAPE will make parallel graph computations accessible to a large group of users who are more familiar with sequential algorithms.

A preliminary implementation of GRAPE is available at [9]. We are in the process of implementing asynchronous message passing, based on [27]. We are also implementing a lightweight transaction controller, to support not only queries but also updates such as insertions and deletions of nodes and edges. When the update load is light, GRAPE adopts non-destructive updates that have
proven useful in functional databases [64]. Otherwise, it switches to multi-version concurrency control [14] that keeps track of timestamps and versions, as adopted by existing distributed systems.

One topic for future work is to revise the asynchronous model of [27] to maximize the benefit of pipelined parallelism and data-partitioned parallelism. Another topic is to develop methods for incrementalizing graph algorithms with performance guarantees, extending [11, 16, 24].

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SUPPLEMENTARY MATERIALS

Proof of Theorem 4.2

(1) Simulate BSP. We first show that all BSP programs can be optimally simulated by GRAPE. Recall that a BSP algorithm $\mathcal{A}$ consists of the following three components: (1) $n$ workers that perform computation of some function $f$; (2) a router that ships data between workers; and (3) a mechanism for synchronizing the computations of the workers [65].

To simulate $\mathcal{A}$, we use PEval and IncEval to simulate the function $f$, and coordinator $P_0$ to play the role of the router. To simulate arbitrary data shipment of BSP, similar to the construction in [27], we construct a complete graph $G_W$ of $n$ nodes as additional input of the BSP program. That is, $G_W$ is a clique of $n$ nodes, which assigns one node $w_i$ to each worker $P_i$ for $i \in [1, n]$, and stores the data transferred to $P_i$ in the status variables of $w_i$, as its update parameters. The reason for using $G_W$ is because in GRAPE, only the update parameters at a worker can be exchanged between workers. By employing $G_W$, all the $n$ nodes become border nodes, and we can simulate the arbitrary data shipment of $\mathcal{A}$ by storing the data in the update parameters of GRAPE workers, and encoding the shipments as messages. The coordinator $P_0$ collects messages from workers, and routes them to the corresponding workers. GRAPE adopts the same synchronization mechanism as BSP.

More specifically, we simulate a given BSP algorithm $\mathcal{A}$ with a PIE program $\mathcal{B}$ as follows.

(a) Data partition: Program $\mathcal{B}$ also uses $n$ workers. It partitions and distributes the input of $\mathcal{A}$ in exactly the same way as $\mathcal{A}$. In addition, as mentioned above, $\mathcal{B}$ takes as input a complete graph $G_W$ of $n$ nodes, which is evenly distributed across the $n$ works, one node designated for each worker.

(b) Update parameters. The update parameters of $\mathcal{B}$ are such defined that they encode the messages transferred by $\mathcal{A}$. That is, for each node $w_i$ in $G$, a status variable $x$ is declared such that $w_i.x$ maintains the data at $P_i$ to be exchanged with other workers.

(c) PEval and IncEval: Both PEval and IncEval of $\mathcal{B}$ are simply the function $f$ of $\mathcal{A}$.

(d) Message grouping. The GRAPE message scheme of $\mathcal{B}$ is used to (i) group the received messages; (ii) distribute the workload to workers. More specifically, the coordinator $P_0$ does the following.

- It first collects all the update parameters for each worker $P_i$ ($i \in [1, n]$).
- It then sends (the changed values of) the update parameters designated to worker $P_i$ ($i \in [1, n]$), in the same way as $\mathcal{A}$ does.

The complete graph $G_W$ allows $\mathcal{B}$ to exchange messages between different workers, i.e., to support point-to-point message passing. The data shipment strategies of BSP can be encoded by the aggregate function of $\mathcal{B}$, to dispatch messages just like $\mathcal{A}$ does.

(e) Assemble: The Assemble function simply collects and returns the partial results from workers.

Given these, one can verify that the PIE program correctly simulates $\mathcal{A}$ under GRAPE. That is, for any input $I$ of algorithm $\mathcal{A}$, $\mathcal{B}$ takes $I$ and $G_W$ as input and returns the same result as $\mathcal{A}$.

Next, we verify that the simulation is optimal. Suppose that given an input $I$, $\mathcal{A}$ runs in $k$ rounds using $T$ time. Suppose that at superstep $r$ ($r \in [1, k]$), $\mathcal{A}$ takes $T_r$ time and sends $C_r$ amount of data. We show that $\mathcal{B}$ also does the job in $k$ supersteps and takes $O(T)$ time. To this end, it suffices to show that $\mathcal{B}$ simulates round $r$ in $O(T_r)$ times, and moreover, it sends $O(C_r)$ amount of data as messages. To see this, observe that when simulating round $r$ of $\mathcal{A}$, $\mathcal{B}$ runs the same function $f$ on the same data, and sends the same data as messages to the coordinator $P_0$ as $\mathcal{A}$ does. The coordinator then routes the message to other workers. Thus $\mathcal{B}$ simulates round $r$ of $\mathcal{A}$ in $O(T_r)$ times, with $O(C_r)$ as its communication cost. Formally, this can be verified by induction on $r$. 

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Putting these together, we can see that GRAPE can optimally simulate BSP.

(2) Simulate MapReduce. It has been shown in [27] that all MapReduce programs using \( n \) processors can be optimally simulated by GRAPE using \( n \) processors. For the completeness of this paper, we also present the construction in [27] here, and provide more details of the proof.

A MapReduce algorithm \( \mathcal{A} \) is specified as follows. The input of \( \mathcal{A} \) is a multi-set \( I_0 \) of \( \langle key, value \rangle \) pairs. The operations of \( \mathcal{A} \) are characterized as a sequence \( (B_1, \ldots, B_k) \) of subroutines, where \( B_r \ (r \in [1, k]) \) consists of a mapper \( \mu_r \) and a reducer \( \rho_r \). Given input \( I_0 \), \( \mathcal{A} \) iteratively runs the subroutines \( B_r \ (r \in [1, k]) \) as follows [22, 43].

(i) The mapper \( \mu_r \) processes each pair \( \langle key, value \rangle \) in \( I_{r-1} \) one by one, and produces a multi-set \( I'_r \) of \( \langle key, value \rangle \) pairs as output.

(ii) Group pairs in \( I'_r \) by the key values. That is, two pairs are put in the same group if and only if they have the same key value. Group \( I'_r \) by distinct keys; this yields \( G_{k_1}, \ldots, G_{k_j} \).

(iii) The reducer \( \rho_r \) processes the groups \( G_{k_l} \ (l \in [1, j]) \) one by one, and produces a multi-set \( I_r \) of \( \langle key, value \rangle \) pairs as output.

(iv) If \( r < k \), then \( \mathcal{A} \) continues to run the next subroutine \( B_{r+1} \) on \( I_r \) in the same manner as steps (i)-(iii); otherwise, \( \mathcal{A} \) outputs \( I_k \) and terminates.

Here \( I_0 \) is the input of \( \mathcal{A} \), and \( I_r \) is the output of \( B_r \ (r \in [1, k]) \). There are two other parameters, namely, \( M_r \) and \( N_r \ (r \in [1, k]) \), which are the numbers of instances of mappers and reducers for each subroutine \( B_r \), respectively. That is, there exist \( M_r \) processors and \( N_r \) processors running \( \mu_r \) and \( \rho_r \), respectively. As put in [43], each mapper (resp. reducer) processes only one \( \langle key, value \rangle \) pair (resp. group) at a time. To simplify the discussion, we assume \( w.l.o.g. \) that each routine uses \( n \) mappers and \( n \) reducers, by reassigning the workload when needed. Generally speaking, there also exists a partition strategy for distributing the outputs of the mappers to the reducers in a MapReduce algorithm. To simplify the discussion, we only consider the hash partition used as default methods in Hadoop [8]. Other partition methods can be simulated similarly.

To simulate the process of the MapReduce algorithm \( \mathcal{A} \) above, we use PEval to simulate the mapper \( \mu_1 \) of \( B_1 \), and IncEval to play the roles of reducer \( \rho_1 \) and mapper \( \mu_1+1 \) in each superstep, for \( i \in [1, k-1] \), and the final reducer \( \rho_k \). Complications arise from the following mismatches: (a) \( \mathcal{A} \) has a sequence \( (B_1, \ldots, B_k) \) of subroutines, while algorithms of GRAPE have only three functions, namely, PEval, IncEval, and Assemble; and (b) \( \mathcal{A} \) groups data by keys and distributes \( \langle key, value \rangle \) pairs across processors, while workers of GRAPE can only exchange the values of update parameters. In a nutshell, to solve problem (a), we define IncEval that takes the subroutines \( B_1, \ldots, B_k \) of \( \mathcal{A} \) as program branches, and makes use of an index \( r (r \in [1, k]) \) to select correct branches via update parameters. We use the status variables of update parameters to store tuples of form \( \langle r, key, value \rangle \) (for \( r \in [1, k] \)), where \( r \) is the index for selecting subroutines in IncEval. GRAPE picks the correct subroutines in IncEval by properly maintaining and citing index \( r \). We solve problem (b) along the same lines as what we do for simulating BSP above, by employing a complete graph \( G_W \) as additional input. We use boarder nodes of \( G_W \) to denote processors, and employ update parameters \( C_{i.x} \) to store associated data.

More specifically, given a MapReduce algorithm \( \mathcal{A} \) with \( n \) processors, we simulate \( \mathcal{A} \) with a PIE program \( \mathcal{B} \) under GRAPE with \( n \) workers. Suppose that the input of \( \mathcal{A} \) is a multi-set \( I_0 \) of \( \langle key, value \rangle \). (a) Data partition: Similar to the simulation of BSP, we construct a complete graph \( G_W \) of \( n \) nodes as additional input of the GRAPE algorithm \( \mathcal{B} \), such that each worker \( P_i \) is represented by a node \( w_i \) for \( i \in [1, n] \). Each node \( w_i \) has a status variable \( x \) to store a multi-set of \( \langle r, key, value \rangle \) tuples. As mentioned above, \( r \) keeps track of different rounds of the computation of \( \mathcal{B} \), for IncEval to select
right subroutines. We distribute the \( \langle \text{key}, \text{value} \rangle \) pairs in \( I_0 \) in exactly the same way as \( \mathcal{A} \) does before running subroutine \( B_1 \); the status variable of each \( w_i \) in \( G_W \) contains the pairs assigned to worker \( P_i \).

(b) Update parameters. As remarked earlier, for each node \( w_i \) in \( G_W \), its status variable \( x \) takes a multi-set of \( \langle r, \text{key}, \text{value} \rangle \) tuples as its value, and the update parameter at worker \( P_i \) is \( w_i.x \).

(c) PEval: PEval simulates mapper \( \mu_1 \) of subroutine \( B_1 \) and organizes its output, as follows.

- Each worker first runs the mapper \( \mu_1 \) of subroutine \( B_1 \) on its local data.
- Next, it prepares the output of \( \mu_1 \) and stores it in the update parameters for later supersteps. Suppose that the output of \( \mu_1 \) is \( I_1' \). For each pair \( \langle \text{key}, \text{value} \rangle \) in \( I_1' \), it includes a tuple \( \langle 1, \text{key}, \text{value} \rangle \) in an update parameter. Here the index 1 in the tuples indicates that these tuples are the results of the mapper \( \mu_1 \).

Note that although we run different subroutines by running subroutine \( B \), running subroutine \( B \) uses the same function \( \text{IncEval} \) as PEval: simulates mapper \( \mu \) of subroutine \( B \) and stores all tuples \( \langle r, \text{key}, \text{value} \rangle \) with the specific \( \text{key} \) in the update parameter of worker \( P_i \).

This is possible since graph \( G_W \) is complete, all the nodes in \( G_W \) are border nodes, and each node in \( G \) denotes a worker. Hence each worker can modify the update parameters of all the other workers.

(d) Message grouping. The coordinator groups and routes messages as follows.

- It first takes a union of the update parameters of all node \( w_i \) \( (i \in [1, n]) \), and then groups the update parameters by the key values.
- Next, to balance the workload, it uses hash partition to assign each tuple \( \langle r, \text{key}, \text{value} \rangle \) to a reducer (i.e., a worker), following Hadoop. More specifically, suppose that \( h \) is the hash function used. Then all tuples \( \langle r, \text{key}, \text{value} \rangle \) with the same \( \text{key} \) will be assigned to worker \( P_j \) with \( j = h(\text{key}) \mod n + 1 \), where \( n \) is the total number of workers, and \( r \in [1, k] \) indicates the round of computation. After this, PEval stores all tuples \( \langle r, \text{key}, \text{value} \rangle \) with the specific \( \text{key} \) in the update parameter of worker \( P_j \).

That is, the \text{aggregateMsg} function groups the \( \langle r, \text{key}, \text{value} \rangle \) tuples by the \text{key} value, and assigns each group to a worker based on hash function \( h \); the group of tuples is sent to the worker as messages and stored in its update parameter.

(e) IncEval. Upon receiving messages from the coordinator \( P_0 \), IncEval first extracts the index \( r \) from the \( \langle r, \text{key}, \text{value} \rangle \) tuples in the messages, and uses the index \( r \) to pick the right subroutine in IncEval. Note that although we run different subroutines by IncEval, GRAPE uses the same function IncEval through the course of the execution. This is done by treating subroutines as branch programs in IncEval, controlled by index \( r \). More specifically, IncEval does the following.

- Extract a multi-set of \( \langle \text{key}, \text{value} \rangle \) pairs from the \( \langle r, \text{key}, \text{value} \rangle \) tuples received. Denote by \( I_r' \) the result of the process.
- On \( I_r' \), run the reducer \( \rho_r \), which can be seen as a branch program of IncEval. Suppose that \( I_r \) is the output of the reducer \( \rho_r \).
- If \( r = k \), i.e., if the reducer \( \rho_k \) has finished the job, then IncEval sets the update parameter of each worker to be empty, which will terminate the algorithm \( B \); otherwise, IncEval runs mapper \( \mu_{r+1} \) on \( I_r \), and generates tuples of the form \( \langle r+1, \text{key}, \text{value} \rangle \) from the output of \( \mu_{r+1} \).

The output is processed in the same way as described in the message grouping part above.

(f) Assemble: The Assemble function simply takes a union of the partial results from all workers.

Having these functions, the PIE program \( B \) simulates \( \mathcal{A} \) under GRAPE as follows. Suppose that \( \mathcal{A} \) runs in \( k \) rounds. Then \( B \) runs in \( k+1 \) rounds, since given a subroutine \( (\mu_r, \rho_r) \) \( (r \in [1, k]) \), \( B \) simulates the mapper \( \mu_r \) in round \( r \), and the reducer \( \rho_r \) in round \( r + 1 \). The extra round is also needed to set parameters empty and terminate the process. By induction on \( k \), one can easily verify that given any input \( I_0 \) of \( \langle \text{key}, \text{value} \rangle \) pairs, \( \mathcal{A} \) and \( B \) produce the same result.
We next show that under GRAPE, the PIE program $\mathcal{B}$ optimally simulates the MapReduce algorithm $\mathcal{A}$. Suppose that given input $I_0$, $\mathcal{A}$ runs in $T$ time, and has communication cost $C$. More specifically, a subroutine $B_r (r \in [1,k])$ takes $T_r$ time, and sends $C_r$ amount of data. To show that $\mathcal{B}$ runs in $O(T)$ time and sends $O(C)$ amount of data, it suffices to show that $\mathcal{B}$ simulates $B_r$ in $O(T_r)$ time, and sends messages of size $O(C_r)$ in the round. To verify this, observe that when simulating $B_r$, $\mathcal{B}$ runs the same functions $\mu_r$ and $\rho_r$ on the same data, except that $\mathcal{B}$ encapsulates the produced $\langle \text{key, value} \rangle$ pairs as $\langle r, \text{key, value} \rangle$ tuples. The update parameters $\langle r, \text{key, value} \rangle$ are generated by the workers in parallel, also in $O(T_r)$ time. In addition, since we only add a number (index $r$) to each key-value pair in the update parameters, $\mathcal{B}$ sends messages of size $O(C_r)$ in the round. Putting these together, we have that $\mathcal{B}$ simulates $B_r$ in $O(T_r)$ time, and incurs communication cost $O(C_r)$ via messages. Hence, $\mathcal{B}$ runs in $O(T)$ time, and sends $O(C)$ amount of data in total.

From the argument above it follows that GRAPE can optimally simulate MapReduce.

(3) Simulate PRAM. Finally, we show that all PRAM programs can be simulated by GRAPE.

PRAM employs a number of processors that share memory, and each processor can access any memory cell in unit time. The computation is typically synchronous. In one unit time, each processor can read one memory location, execute a single operation and write into one memory location. PRAM is further classified by various access policies of shared memory, e.g., CREW PRAM indicates concurrent read and exclusive write (see [66] for details).

It is known that a CREW PRAM algorithm using $t$ time with $O(P)$ total memory and $O(P)$ processors can be simulated by a MapReduce algorithm in $O(t)$ rounds using at most $O(P)$ reducers and memory [43]. By Theorem 4.2(2) above, each MapReduce algorithm in $r$ rounds can be simulated by GRAPE in $r + 1$ supersteps. From these Theorem 4.2(3) follows. □

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