GRAHOPT: constrained-optimization-based parallelization of irregular graphs

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Abstract—Sparse, irregular graphs show up in various applications like linear algebra, machine learning, engineering simulations, robotic control, etc. These graphs have a high degree of parallelism, but their execution on parallel threads of modern platforms remains challenging due to the irregular data dependencies. The execution performance can be improved by efficiently partitioning the graphs such that the communication and thread synchronization overheads are minimized without hurting the utilization of the threads. To achieve this, this paper proposes GRAHOPT, a tool that models the graph parallelization as a constrained optimization problem and uses the open Google OR-Tools solver to find good partitions. Several scalability techniques are developed to handle large real-world graphs with millions of nodes and edges. Extensive experiments are performed on the graphs of sparse matrix triangular solves (linear algebra) and sum-product networks (machine learning), respectively, showing a mean speedup of 2.0× and 1.8× over previous state-of-the-art libraries, demonstrating the effectiveness of the constrained-optimization-based graph parallelization.

Index Terms—graph parallelization, partitioning, constrained optimization, sparse matrix triangular solves, CPU multithreading

1 INTRODUCTION

Significant advances have been made in accelerating massively parallel computations like image processing and deep neural networks, which typically involve regular memory accesses and well-structured explicit parallelism. These advances can be ascribed to dedicated programming frameworks like Tensorflow [1] and Halide [2], optimized compilation approaches like polyhedral compilation [3], and specialized hardware architectures like GPU and TPU. However, these approaches cannot be readily extended to another equally important class of parallel applications that is irregular. Such applications involve irregular memory accesses lacking any apparent recurring patterns, and parallelism that is difficult to partition. Such computations arise in applications like graph workloads, sparse linear algebra, probabilistic machine learning, recommender systems etc.

A subset of these irregular applications can be represented as static directed acyclic graphs (DAG), where the nodes represent operations to perform and edges represent data dependencies among these operations. These DAG workloads can be further classified into two categories: 1) coarse-grained and 2) fine-grained, as shown in fig. 1. The coarse-grained DAGs, although irregular, have as their nodes large regular operations like dense tensor operations. The computation within each node is enough to amortize parallelization costs associated with thread synchronization, inter-thread communication, GPU kernel launch, etc. The examples of coarse-grained graphs include neural networks and linear algebra with block/structured sparsity, graph neural networks, visual rendering, electronic circuit placement, video encoding etc. These applications can be accelerated efficiently using frameworks like Tensorflow, TaskFlow

Fig. 1. DAG structures and granularities. Illustration of regular, coarse-grained irregular, and fine-grained irregular compute graphs

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1. Available at https://github.com/nimish15shah/GRAPHOPT

• Intel Thread Building Blocks (TBB) [5] etc., by modeling nodes as individual tasks.

On the other hand, nodes in fine-grained DAGs represent only a couple of scalar operations, whose computation cost cannot amortize synchronization and task launch overheads when each node is modeled as an individual task. As a result, these DAGs cannot be accelerated by simply modeling them as task graphs in Tensorflow, etc. Their acceleration needs the creation of coarser partitions by combining original fine-grained nodes, to increase computation to synchronization/communication ratio. But if the partitions become too coarse, they hurt parallelism as there might not be enough partitions available to execute in parallel. Hence, appropriate granularity and parallelism of the partitions are critical for good acceleration. To this end, this paper proposes GRAHOPT—a partitioner to efficiently parallelize fine-grained DAGs through hardware-aware partitioning.
The paper is organized as follows. Section §2 defines the key contributions of the paper are as follows:

- **Context:**

  - **GRAPHOPT** models the graph partitioning for parallel execution as a constrained optimization problem, and leverages a state-of-the-art solver.
  - Several scalability techniques are proposed to handle real-world graphs with millions of nodes and edges.
  - The performance of GRAPHOPT is validated for two applications: 1) sparse matrix triangular solves from linear algebra and 2) sum-product networks from machine learning, and compared against standard libraries.

The paper is organized as follows. Section §2 defines the problem of parallelizing fine-grained DAGs and GRAPHOPT's approach. Section §3 details the working of GRAPHOPT, followed with extensive performance benchmarking in section §4. Finally, section §5 discusses related works and section §6 concludes the paper.

## 2 GRAPH PARTITIONING FOR PARALLELIZATION

Modern computing platforms like multi-core CPUs and GPUs are equipped with parallel hardware threads, which can execute DAG nodes in parallel. However, the nodes cannot be arbitrarily scheduled because of the data dependencies represented by the DAG edges, i.e., a node can only be executed after all the predecessor nodes have finished their execution. This data dependency demands threads synchronization when a predecessor node is mapped to a different thread than the current one. Furthermore, the nodes in raw fine-grained DAGs do not have enough computation to be executed as a stand-alone task in a task-scheduling framework (like Intel TBB [5], etc.) because of the task-launch and synchronization overheads. This can be addressed by clustering the nodes in coarser partitions that are executed as monolithic tasks to amortize the overheads. The quality and correctness of these coarser partitions depend on several aspects as discussed next (with illustrations in fig. 2).

### Data dependencies and acyclic partitions

The data dependencies of DAG edges imply that a partition can be launched as a monolithic unit only if all the predecessor partitions have finished the execution. Furthermore, the edges between partitions should not create cycles, because cyclic partitions need intermittent synchronization to resolve intermediate data dependencies. The cycles can be prevented by generating convex partitions, i.e., if two nodes are in a partition, the nodes on all the (directed) paths in between the two nodes also have to be in the partition. An example of cyclic partitions is shown in the fig. 2(d). GRAPHOPT avoids these cycles by enforcing an acyclic constraint.

### Granularity and parallelism

The sizes of the partitions dictate how often the threads need to synchronize and communicate. To reduce the overall runtime, there are multiple, conflicting, requirements:

- Partitions should be as large as possible to amortize the overheads and increase the local data reuse, minimizing communication across threads. For example, increasing the granularity in fig. 2(c) and (e) helps.
- There should be enough parallel partitions to keep all the available threads in the underlying hardware busy. Partitions in fig. 2(a) and (b) do not have any parallelism across threads at all.
- Partitions that are supposed to execute in parallel should be of similar size to balance the workload across threads. Figure 2(c) shows a counter-example.

These requirements suggest that the partition granularity depends on the parallelism of the underlying hardware like the number of CPU threads, which is fixed and known beforehand. It also depends on the available parallelism in the DAG, which can vary in the different parts of the DAG. Hence, the partition granularity cannot be manually fixed but has to be automatically adjusted depending on the DAG structure. GRAPHOPT achieves a balance by generating partitions that are as large as possible, as long as there are enough parallel partitions.

### Communication

An edge from one partition to the other indicates communication of data. If the two partitions are executed on the same thread, the data can be locally reused via local caches or scratchpads. Whereas, the communication across threads incurs a higher overhead of flushing data to the shared caches. This communication overhead can be reduced by keeping the edges within the same thread as much as possible. Figure 2(e) shows an example where partitions can be simply remapped to different threads to avoid inter-thread communication.

### GRAPHOPT's approach

To appropriately handle the various trade-offs, instead of creating arbitrary partitions, GRAPHOPT creates a layered graph of coarse partitions as shown in fig. 3. To avoid confusion, a layer of coarse partitions is always referred to as a super layer in the rest of the paper, and a layer simply means a layer of nodes in the original fine-grained DAG. Every super layer has $P$ independent partitions, where the user can specify an
3 GRAPHOPT

This section explains the generation of super layers with \( P \) parallel, balanced, coarse partitions from a fine-grained DAG. The optimal graph partitioning, even without the acyclic constraint and parallelism requirement, is known to be NP-complete \([6, 7]\). Recent work \([8]\) has shown that graph partitioning with the acyclic constraint is also NP-complete. Section 3.1 explains why general graph partitioning approaches cannot be used here because of the parallelism requirement (\( P \) independent partitions) and the acyclic constraint. These general approaches only focus on minimizing edges among (possibly cyclic) partitions, and do not aim to generate layered graphs with \( P \) parallel workload-balanced partitions needed to keep parallel threads busy.

Figure 3 shows GRAPHOPT’s approach for generating partitioned super layers. To reduce the complexity, instead of finding all the super layers simultaneously, the tool iteratively constructs one super layer at a time going from the bottom to the top. In an iteration, a super layer is generated with two main steps: (M1) recursive two-way partitioning and (M2) workload-balancing. The S1, S2, and S3 are the scalability techniques that enable GRAPHOPT to handle large graphs with millions of nodes/edges.

An iteration starts by selecting a part of the DAG that is considered for generating the current super layer. Ideally, all the currently unmapped nodes should be considered, but to limit the complexity, step S1 selects a subgraph \( G \) from the unmapped DAG. The M1 step splits this subgraph \( G \) into \( P \) parallel partitions and associates them to the \( P \) underlying hardware threads. These partitions, however, could potentially be of different sizes. The M2 step redistributes nodes among these partitions for workload balancing, generating \( P \) balanced partitions for the current super layer. The unmapped nodes that could not be mapped to any partitions are then considered for the subsequent super layers.

3.1 Recursive two-way partitioning (M1)

Given a subgraph \( G \), a super layer with parallel partitions should ideally be constructed by a direct \( P \)-way partitioning. GRAPHOPT relaxes this by using recursive two-way partitioning, i.e. recursively splitting subgraphs into two parallel smaller subgraphs until getting \( P \) subgraphs (partitions) for \( P \) threads, as illustrated in fig. 3(top). The recursion starts with the aim of mapping the input subgraph \( G \) to \( P \) threads. The first two-way partition generates two output partitions, one of which represents the nodes corresponding to \( t_1, \ldots, t_{P/2} \) threads, and the other corresponding to \( t_{P/2+1}, \ldots, t_P \) threads. The third output is a set of unmapped nodes that cannot be mapped to either partition without adding an edge between the partitions. These unmapped nodes will be considered for the subsequent super layers. The next recursion splits the first partition (which becomes the current \( G \)) into two smaller partitions, one for \( t_1, \ldots, t_{P/4} \) threads and the other for \( t_{P/4+1}, \ldots, t_{P/2} \) threads. This repeats until partitions for individual threads are determined. Thus the problem of one super layer generation is reduced to multiple iterations of two-way partitioning under given constraints and objectives. Note that if \( P \) is not a power of 2, the partitions can end up being imbalanced, which is addressed with the M2 step.

Instead of developing a custom heuristic algorithm, GRAPHOPT models the two-way partitioning problem with the Minizinc constrained-optimization language \([10]\). Such a model can be solved with state-of-the-art constraint programming (CP) or mixed-integer linear programming.
Given an input graph, the two-way partitioning aims to allocate the nodes to two parallel partitions such that there is no edge crossing from one to the other. Furthermore, the size of the partitions should be as large and equal as possible. If the target for the current recursion are \(t_1, t_2, \ldots, t_x\) threads, the first output partition corresponds to \(t_1, \ldots, t_{x/2}\) threads and other to \(t_{x/2+1}, \ldots, t_x\) threads. The inter-thread communication (blue edges in fig. 3) would reduce if the sources of the incoming edges of the partitions are from the same group of threads. Hence, one of the aims of the two-way partitioning is also to perform allocation such that the nodes in the first partition mostly have incoming edges from \(t_1, \ldots, t_{x/2}\) threads, and the second partition from \(t_{x/2+1}, \ldots, t_x\) threads.

Table 1 shows different parts of the optimization model. The current input DAG is denoted by \(G(V, E)\), where \(V\) is the set of nodes (vertices), and \(E\) is the set of directed edges. Note that this is not the complete original DAG, but an input subgraph for the current recursion of the two-way partitioning. The output partitions of \(G\) are decided by the decision variable \(PART(V)\), an array of integers, one for every node. If \(PART[v] = 1\) or 2, the node \(v\) is allocated to the partition 1 or 2 respectively, and if \(PART[v] = 0\), it is not allocated. The constraints and objectives are discussed next.

**Notations**: \(\forall\) for all, \(\in\) is member of, \(||\) such that, \(\lor\) logical or, \(\land\) logical and, \(\lfloor\rfloor\) floor function.

**Acyclic and data-dependency constraint**
There should not be any edge from one partition to the other, which implies that, for the destination and source nodes of every edge, \(PART[dst]\) should either be equal to \(PART[src]\) or should be 0. This also ensures that the destination node is unallocated if the source node is also unallocated, which is needed because the edges represent data-dependencies. This constraint is modeled as follows,

\[
\forall (src, dst) \in E, \\
PART[dst] = PART[src] \lor PART[dst] = 0 \quad (1)
\]

**Partition size constraint**
The input parameter \(node\_w(V)\) (array of integers) represents the amount of computation to be performed in each node. For workload balancing, the amount of computation in the two partitions should be the same. To formulate such an optimization objective, the decision variables \(PART\_1\_size\) and \(PART\_2\_size\) are used, which are modeled with the following constraint,

\[
\forall v \in V, \\
PART\_1\_size = \sum(node\_w[v] \mid PART[v] = 1) \\
PART\_2\_size = \sum(node\_w[v] \mid PART[v] = 2) \quad (2)
\]

**Inter-thread communication constraint**
The blue edges in fig. 3 contribute to inter-thread communication. An edge would become a blue edge if its source node is already allocated in a previous super layer to a thread \(t_a\), and the destination node is currently allocated to a partition that does not correspond to \(t_a\). Note that these edges are not in the current edge set \(E\), because the edges in \(E\) have the source and destination nodes that are being considered for the current super layer. Another input to the model \(E_{in}\) represents such edges, which have source nodes (represented

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**3.1.1 Optimization model for the two-way partitioning**

(MILP) solvers like Google OR-Tools [9], SCIP [10], Gurobi [11] etc. These solvers are designed and tuned with decades of research and often outperform custom heuristics for smaller problem instances, but struggle to scale to larger problems. This is addressed in this work by developing the scalability techniques explained later in sec. 3.3. An optimization model consists of four parts: 1) inputs of the problem, 2) decision variables whose values need to be determined by the solver, 3) constraints on the decision variables, and 4) the objective of the optimization (refer [13] for more details of constrained optimization). The rest of the section describes these four parts.

![Fig. 5. The recursive two-way partitioning (M1) uses a Minizinc-based optimization model to partition subgraphs until getting P partitions. Due to the recursive approach, the partitions can be imbalanced. The workload balancing (M2) iteratively redistributes the nodes, using the same Minizinc-based model, to generate a balanced super layer.](image-url)
TABLE 1
Optimization model. Inputs, decision variables, constraints, and objective of the Minizinc two-way partitioning optimization model

| Name | Description | Type |
|------|-------------|------|
| | Target threads for this recursion | array of int |
| V | Set of nodes in the current DAG G | set of int |
| E (V, V) | Set of directed edges in G expressed as tuples of source and destination nodes | set of int tuples |
| node_w (V) | Weights indicating the amount of computation within nodes | array of int |
| V_in | Set of nodes that are already allocated to previous super layers | set of int |
| E_in (V_in, V) | Set of directed edges with source node in V_in and destination in V | set of int tuples |
| PART_in (V_in) | Allocated partitions of nodes in V_in | array of int in [1, 2] |

Decision variables: Final output

| PART (V) | Allocated partitions for nodes in V, where 0 indicates no allocation | array of int in [0, 2] |

Decision variables: Intermediate

| PART_1_size | Amount of computation allocated to partition 1 | int |
| PART_2_size | Amount of computation allocated to partition 2 | int |
| E_in_crossing (E_in) | Indicates whether the edge in E_in are crossing partitions or not | array of bool |

Constraints

| Acyclic parts | ∀(src, dst) ∈ E, PART[dst] = PART[src] ∨ PART[dst] = 0 |
| Partition size | ∀v ∈ V, PART_1_size = sum(node_w[v] | if PART[v] = 1), PART_2_size = sum(node_w[v] | if PART[v] = 2) |
| Inter-thread comm. | ∀(src, dst) = e ∈ E_in, E_in_crossing[e] = ((PART[dst] ≠ 0) ∧ (PART[dst] ≠ PART_in[src])) |

Objective

maximize \( w_s \times \min(\text{PART}_1\text{size}, \text{PART}_2\text{size}) - w_c \times \sum(E_{in}\text{crossing}) \)

by the set \( V_{in} \) in the previously generated super layers, and destination nodes in the current \( G \). Input \( \text{PART}_\text{in}(V) \) represents the partitions of the nodes in \( V_{in} \) based on the threads they are allocated to. If a \( v_{in} \) was allocated to any of the threads \( t_1, ..., t_{x/2} \) in the previous super layers, \( \text{PART}_\text{in}[v_{in}] = 1 \), and if allocated to any of the \( t_{x/2+1}, ..., t_x \) threads \( \text{PART}_\text{in}[v_{in}] = 2 \). If a \( v_{in} \) was not allocated to any of the current target threads \( t_1, ..., t_x \), its corresponding edges always result in inter-thread communication irrespective of how the current partitioning is done. Hence, such \( v_{in} \) and the corresponding edges are not considered in the model.

An edge in \( E_{in} \) is a crossing edge when the partitions of the destination and source nodes are different. The edge crossings are tracked with \( E_{in}\text{crossing} \) (array of booleans), modeled with the following constraint,

\[
\forall (src, dst) = e \in E_{in}, E_{in}\text{crossing}[e] = ((\text{PART}[dst] ≠ 0) \land (\text{PART}[dst] ≠ \text{PART}_\text{in}[src]))
\]  

(3)

The first inequality makes sure that the edges with unallocated destination are not marked as crossing edges.

Objective

The objectives of \text{GRAPHOPT} are maximizing but also equalizing the partition sizes and minimizing the edge crossings. The optimization solvers generally support only one objective, hence a weighted sum of the multiple objectives is used. The objective makes sure the smaller of the two partitions is made as big as possible.

maximize \( w_s \times \min(\text{PART}_1\text{size}, \text{PART}_2\text{size}) - w_c \times \sum(E_{in}\text{crossing}) \)

(4)

Typically, global synchronization cost is significantly higher than communication cost (i.e., accessing data from other core’s cache), the hyperparameter \( w_s \) should be set higher than \( w_c \). In our experiments, \( w_s \) is set to \( 10 \times w_c \). The objective along with the constraints in the equations form the Minizinc optimization model, which is solved with the Google OR-Tools solver.

3.1.2 Example

The figure illustrates the optimal two-way partitioning of a simple \( G \). The nodes set \( V \) is \{1, ..., 9\} and the edge set \( E \) is \{(1,5), (2,5), ..., (8,9)\}. The computation in every node, the \( \text{node}_w \), is assumed to be 1. Assume that the target threads are \{\( t_1, ..., t_4 \)\}. The incoming edges \( E_{in} \) are \{(10,1), (10,7), ..., (13,4)\} and suppose their source nodes \( V_{in}, \{10, ..., 13\} \) are mapped to the threads \{\( t_2, t_3, t_4, t_5 \)\} respectively, in the previous super layers. Hence, \( \text{PART}_\text{in}[10] = \text{PART}_\text{in}[11] = 1 \), and \( \text{PART}_\text{in}[12] = \text{PART}_\text{in}[13] = 2 \).

The variable \( \text{PART}[9] \) for the top node will remain 0, otherwise due to the constraint in the eq. all the nodes would end up in the same partition (which would be a valid but suboptimal solution). The \( \text{PART} \) for the other nodes are decided such that the \( E_{in}\text{crossing} \) (blue edges) are minimized. Switching the \( \text{PART} \) of 1,2,5,7 with 3,4,6,8 would lead to more blue edges. Hence, the solution shown in the figure is the optimal solution. In one of the next recursions, \( G \) will contain \{1,2,5,7\} nodes with the target threads \{\( t_1, t_2 \)\}. And the other recursion will be with \{3,4,6,8\} nodes and target threads \{\( t_3, t_4 \)\}. Node 9 is an unmapped node, which will return to the set of remaining nodes to be used in the construction of the next super layer.
3.2 Workload balancing (M2)

A penalty of using recursive two-way partitioning instead of a direct $P$-way partitioning is that the $P$ partitions are not guaranteed to have the same size. The two-way partitioning attempts to equalize the partition sizes, but this does not guarantee equal parallelism. This imbalance can lead to divergences in partition sizes in subsequent recursions. Moreover, the imbalance can also occur when $P$ is not a power of 2. To address this, a workload balancing step (M2) is used as shown in fig. 5(bottom), which redistributes the nodes across imbalanced partitions. In every iteration, the partitions are sorted according to the sizes. The nodes of the largest and the smallest partitions are combined and two-way repartitioned (with the Minizinc model) in an attempt to redistribute the workload. This repeats until the size of the smallest no longer increases further. If the sizes are still unequal, the larger partitions are truncated in topological order to equalize the sizes (with some margin). The truncated nodes will be added to the pool of unmapped nodes to be considered for the next super layer. The final output of this step is a super layer with balanced $P$ partitions.

3.3 Scale to large graphs (S1, S2, S3)

The two-way partitioning model can handle graphs with tens of thousands of nodes and edges in a reasonable time. Hence, the M1 and M2 steps explained earlier are sufficient to generate super layers for such graphs. However, graphs from real applications can have millions of nodes/edges, making the solver runtime prohibitively long. GRAPHOPT uses several techniques to handle the complexity of such large graphs, as shown in the full flow in fig. 7.

Consider limited layers (S1)

Ideally, all the unmapped nodes of the DAG should be considered for allocation in every iteration of super layer generation. However, during the partitioning for initial $bottom$ super layers, it is unlikely that the nodes from the $top$ of the graph will be allocated. Hence, it is wasteful to consider the entire unmapped graph for the partitioning, and the complexity can be limited by choosing a subset $G$. With this aim, each node in the graph is assigned to a layer number before beginning the generation of super layers, using the “as last as possible” heuristic, such that every node is in one layer below its lowest successor node. This heuristic only needs a topological sort of graph nodes, which runs in $O(|V| + |E|)$ (i.e., linear in the size of $G$) time. In every iteration, GRAPHOPT adaptively considers a limited number of layers of the unmapped graph, chosen such that the input graph $G$ for the M1 step has size $\alpha$ (set to 4 in our experiments) times the size of the output super layer in the previous iteration. This automatically chooses an appropriate sized $G$ depending on the parallelism in the DAG. A high $\alpha$ leads to better super layer quality at the expense of partition time, and vice-versa.

Independent connected components (S2)

During the two-way partitioning in M1 and M2, the current $G$ to partition may not be a fully connected graph, but may have multiple disconnected components. This can simplify the partitioning because disconnected components, by definition, do not have edge crossings. Hence, each component is successively considered as current $G$ and partitioned with the solver independently. Suppose the target for the current recursion is $Y$ threads, then the components are partitioned with a target of $X$ threads, chosen as,

$$X = \left\lfloor \frac{Y \times \text{size of the current component}}{\text{size of all components}} \right\rfloor.$$

These independent connected components are discovered using a breadth-first search, running in $O(|V| + |E|)$ (i.e., linear in the size of $G$) time.

Heuristic coarsening (S3)

Even with the S1 and S2 techniques, a large graph may have to be two-way partitioned. If the graph is larger than a threshold $thresh_G$, a list-based heuristic coarsening is used before the partitioning. The graph nodes are sorted in a list according to the depth-first traversal order as shown in fig. 8, which runs in $O(|V| + |E|)$ (i.e., linear in the size of $G$) time. During the traversal, the differences in depth between subsequent nodes are also noted in a list. The third list indicates the out-degree for each node. The node list is then broken into clusters according to the following criteria:

- The size of the cluster should be less than a $size_{threshold}$. In the example, cluster 1 is stopped at node 7 for the $size_{threshold}$ of 4.
- The difference in depth among consecutive nodes should be less than a $depth_{threshold}$. Eg., the difference in depth for the consecutive nodes 7 and 3 is high, so cluster 1 should be stopped at node 7 according to the depth difference as well.
- Clusters should be stopped at the nodes with out-degree higher than a $degree_{threshold}$. Eg., cluster 2 is stopped at node 6 if the $degree_{threshold}$ is 2.

A coarse graph is constructed with these clusters, which will be used as the current $G$ for two-way partitioning. The clusters are represented as a single node in the coarse graph with a node weight (amount of computation) equal to the sum of all the enclosing node weights. If the resulting graph is very coarse, then it may adversely affect the quality of the subsequent two-way partitioning. As such, the size threshold is chosen according to the current graph size, resulting in a coarse graph with around 1000 nodes (empirically found...
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Fig. 7. The full flow with S1, S2, and S3 scalability steps that enables the GRAPHOPT to handle large graphs with millions of nodes/edges.

Fig. 8. The data structures generated by depth-first traversal for the heuristic coarsening step (S3).

4 PERFORMANCE EVALUATION

4.1 Workloads

The multi-threaded CPU performance of GRAPHOPT is evaluated for DAGs from two applications: 1) Sparse matrix triangular solves of linear algebra, and 2) Sum-Product Networks of probabilistic machine learning.

4.1.1 Sparse matrix triangular solves (SpTRSV)

Matrix triangular solve is a fundamental operation needed to solve linear system of equations \( Lx=b \), where \( L \) is a lower (or upper) triangular matrix and the vector \( x \) is evaluated for a given vector \( b \) [14]. This operation has wide-ranging use in engineering simulations, structural analysis, power systems analysis, economics, control, etc. The matrices arising in real-world problems typically turn out to be sparse, i.e. most of the matrix elements are zero. For example, in electric circuit simulations, a matrix can represent the connectivity of a circuit, with rows/columns indicating the circuit nodes and the matrix elements indicating whether two nodes are connected. Since real-world circuit nodes are typically connected to only a few other nodes, such a connectivity matrix will be sparse. Furthermore, in many applications the sparsity pattern of the matrix remains identical across multiple triangular solves (e.g. the electric circuit structure may remain the same across simulations), providing the opportunity to perform extensive partitioning to improve the runtime performance.

The computation of the triangular solve can be represented with a DAG, where each node represents a row, and
Fig. 9. Detailed analysis of super layers. Row (f) shows that DAGs can be partitioned into a few, large super layers. It also shows the size of the original DAG layers for comparison. Row (g) shows the workload balancing across threads, in the form of operations in different threads in super layers. Row (h) shows the throughput scaling with parallel threads, demonstrating the advantage of using super layers versus direct DAG-layer partitioning. Rows (i) and (j) show the improvement in partitioning time due to scalability techniques S1, S2, and S3.

the node weight is equal to the number of corresponding multiply-accumulate (MAC) operations. If a matrix element $L[i,j]$ is non-zero, the DAG contains an edge from node $j$ to node $i$, indicating a data dependency. The numbers of DAG nodes and edges are the same as the number of rows and non-zero elements in the matrix, respectively.

4.1.2 Sum-Product Networks

Sum-Product Networks (SPN, more generally called a probabilistic circuit) [15], [16] is a machine learning workload that can tractably model joint probabilities of random variables. SPNs are often used in combination with neural networks, for various reasoning and perceptual tasks like noise-tolerant image recognition [17], robotic navigation [18], robust human-activity detection [19], etc. The SPN is a DAG of sum and product operations that can compute complex probabilistic inferences like the marginal and conditional probability of the random variables. The DAG structure is often irregular and remains unchanged during the inference, making it a good candidate for GRAPHOPT.

In addition to these workloads, sparse lower-upper (LU) decomposition and Cholesky decomposition for applications with fixed sparsity structure but changing numerical values (e.g. circuit simulation [20]) are also good candidates for parallelization with GRAPHOPT.

4.2 Experimental setup

Experiments are conducted on the matrices from the SuiteSparse matrix collection [21] of real-world applications like power network optimization, structural analysis, computational fluid dynamics, non-linear optimization, economics, robotics, etc. The SPNs from a standard benchmark [22] are used for evaluation. The super layers generated from the GRAPHOPT are parallelized across multicore CPU threads using OpenMP. The throughput results are averaged over 1000 iterations on up to 18 threads on an
Intel® Xeon Gold 6154 CPU with 18 cores, with GCC v4.8.5 compiler, -march=native -Ofast flags, and the thread affinity set as KMP_AFFINITY = granularity = fine,compact,1,0. The experiments with 18 threads are adequate for the target workloads because the workloads have a mean parallelism (quantified as total nodes in a DAG / critical path length) of 8.6, and 95% of the DAGs achieve peak throughput with fewer than 18 threads. The caches are warmed up by executing the same program before the actual measurement.

4.3 Analysis of super layers

Several experiments are conducted on workloads of varying sizes to evaluate the different properties of super layers, as summarized in fig. 9.

4.3.1 How large are the super layers?

GRAPHOPT combines nodes from multiple DAG layers to create large super layers. The row (f) in fig. 9 shows the number of multiply-accumulate operations in super layers compared to the original DAG layers. GRAPHOPT manages to compress thousands of DAG layers into tens of super layers, reducing the required synchronization barriers.

4.3.2 Workload balancing

Large super layers reduce the number of synchronizations, but good parallel performance demands that the workload is also balanced across threads. The row (g) in fig. 9 shows the number of operations in each super layer for $P$ equals to 2 and 8 threads. As seen, GRAPHOPT balances the workload across parallel partitions in a super layer as much as possible. Also note that the granularity of partitions varies across different super layers, depending on the available parallelism in the corresponding DAG region.

4.3.3 Throughput scaling

The row (h) shows the scaling of throughput with parallel threads. Different matrices reach peak throughput with different preferred threads depending on the parallelism in the DAGs. For comparison, the throughput of direct “DAG layer partitioning” is shown in the orange curve. In this partitioning, the nodes of a single DAG layer are executed in parallel across threads, and the threads are synchronized after every layer. The DAG layers are created with the multi-frontal UMFPACK V5.7.9 [24] algorithms from the widely-used SuiteSparse software collection V5.8.1. The UMFPACK routine is used in Matlab.

4.3.4 Impact of the scalability techniques

To see the impact of S1 to S3 scalability techniques on the partitioning time, the partitioning is performed with and without these techniques, with a timeout of 1 hour. Figure [9](i) and (j) shows that the tool times-out for the larger graphs without these techniques.

4.4 Comparison with state-of-the-art libraries

4.4.1 Sparse matrix triangular solves

As shown in fig. 10, the performance of state-of-the-art libraries is evaluated on the L triangular factor DAG of 370 matrices from the SuiteSparse matrix collection [21], with selection criteria that the matrices should be real, square, non-singular, and with <50M non-zeroes in the resulting LU factors (to limit the duration of the experiments). The experimental details are as follows.

- This work: GRAPHOPT is used to generate super layers with $P$ set to 2, 4,..., 18 parallel threads.
- SuiteSparse: Performance of the CXSparse V3.2.0 [23] and the multi-frontal UMFPACK V5.7.9 [24] algorithms from the widely-used SuiteSparse software collection V5.8.1. The UMFPACK routine is used in Matlab.
- Intel MKL: The mkl_sparse_s_trsv() sparse routine from the Intel Math Kernel Library (MKL) V2021.1 [25] is benchmarked for comparison.
- DAG layer partitioning: This is the same as the orange partitioning in fig. 9 which is a common heuristic approach used in several libraries. The nodes of a DAG layer are executed in parallel across threads (which is possible because, by definition, there are no edges within nodes in a layer), and all the threads are synchronized after every layer. The DAG layers are created with the as-late-as-possible (ALAP) heuristic, such that every node is allocated to one layer below its lowest successor node (same as the heuristic used in the S1 step in §3.3).
- Point-to-Point (P2P): Based on [26] that also uses the DAG layer partitioning, but instead of using global barriers, specialized point-to-point sparsified barriers are used for only the threads involved in dependencies, avoiding unnecessary stalls of the rest of the threads.
- KokkosKernels: Performance of the sparse kernels from the portable Kokkos library V3.4.1 [27] is benchmarked.

Results: As shown in fig. 10 the GRAPHOPT outperforms the next best implementation, SuiteSparse CXSparse, on matrices with >10k nonzeroes. For smaller matrices, SuiteSparse CXSparse reports the highest performance. Overall, GRAPHOPT achieves mean speedups of 2.0, 3.3, 3.1, 5.6, 10.8, and 23.7 over SuiteSparse CXSparse, Intel MKL, SuiteSparse UMFPACK, P2P, DAG layer partitioning, and KokkosKernels, respectively. The main contributor for the speedup is fewer synchronization barriers (99% reduction compared to the DAG layer partitioning).
4.4.2 Sum-Product Networks

Fig. 11 shows the throughput for 16 SPNs from the standard benchmark [22] achieved with following implementations.

- **This work**: GRAPHOPT is used to generate super layers with $P$ set to 2, 4, ..., 18 parallel threads.
- **DAG layer partitioning**: Same as the sparse triangular solve experiment in section 4.4.1
- **Juice**: Performance of Juice — a widely-used Julia-based library for SPNs [28].

**Results**: Juice library, despite of using the layer-based partitioning scheme, achieves significantly lower throughput than the OpenMP-based DAG layer partitioning implementation. GRAPHOPT achieves a mean speed-up of 1.8 and 1052 over DAG layer partitioning and Juice, respectively, due to 88.5% fewer synchronization barriers.

5 DISCUSSION AND RELATED WORK

5.1 Sparse triangular solves

A common approach for parallelizing triangular solves is the DAG layer partitioning method that partitions nodes on each DAG layer directly into $P$ partitions, and synchronizes the threads after every layer, first introduced in [29]. This is one of the baselines in the experiments section. This partitioning is quicker than our approach when the sparsity pattern/DAG structure changes for every triangular solve. However, for large matrices, thousands of synchronizing barriers might be needed depending on the critical path length of the DAG, incurring large overhead. As shown in our experiments, 99% barriers can be avoided by combining multiple DAG layers into super layers, improving the throughput significantly compared to the DAG layer partitioning (fig. 10). The point-to-point (P2P) barrier approach alleviates some overhead of the global barrier as shown in fig. 10 but still fails to outperform other libraries.

The works in [30] and [31] are the most similar to this paper, but could not be compared due to the unavailability of open-source code. These works have two key conceptual differences with our work:

1) Both the papers limits the partition sizes. In [30], the partitions should fit in the local scratchpads of GPU, while in [31], the size is controlled with a predefined hyperparameter that has to be tuned for every DAG. This hyperparameter remains the same for the entire DAG even when the local parallelism can vary in different parts of the DAG. This is in contrast with our approach of making the partitions as large as possible as long as there are $P$ parallel partitions. In other words, by explicitly defining the hardware parallelism (via $P$), GRAPHOPT automatically adjusts the partition sizes based on the available parallelism in the DAG, reducing the overall number of partitions and global barriers.

2) Without [30] and [31] develop a partitioning heuristic, while GRAPHOPT uses constrained optimization and leverages a state-of-the-art solver, which often achieve better solutions than custom heuristics.

5.2 Sum-Product Networks

The DAG layer partitioning heuristic is used for SPN for CPU, GPU and a custom ASIC parallelization [25, 32, 33]. Our experiments show a speedup of 1052× over Juice [28]. Libraries based on Tensorflow have also been developed for coarse-grained SPNs with explicit regular structures [34, 35]. However, such a Tensorflow-based approach is not useful for fine-grained, irregular SPNs due to the overheads of kernel launch etc. GRAPHOPT does not assume any regularity in SPN structure.

5.3 Graph partitioning

As explained in section 5, GRAPHOPT essentially needs to P-way independent partitioning of a directed graph while ensuring that resulting partitions are acyclic and balanced. In general, graph partitioning is known to be NP-complete [6, 7] and is a widely studied problem. Several partitioning algorithms have been developed [36, 37, 38], but they only focus on undirected graphs intending to reduce the edge crossings within balanced partitions, while ignoring the edge direction. As a result, the popular undirected partitioning software like JOSTLE [39] and METIS [7] cannot be used for acyclic partitioning.

The acyclic partitioning of DAGs is also shown to be NP-complete like the undirected version of the problem [8]. In recent years, several works have been proposed to tackle the problem [8, 40, 41, 42]. However, these works do not focus on parallelism. The resulting partitions would be acyclic, well-balanced, with minimal edge crossings, but can end up being completely sequential, i.e. only one partition can be executed at a time. This stems from the fact that the usual objective of minimizing edge crossings does not guarantee parallelism. Hence, these methods are not suitable for parallelizing a DAG execution over multiple threads.

Several algorithms have been proposed for scheduling DAGs [43, 44, 45], which use either list-based or clustering-based scheduling heuristics, while GRAPHOPT takes a different approach of modeling the core routine of
the tool as a constrained-optimization problem, allowing the use of open-source solvers. The constrained optimization-based approach is explored in [45], [47]. However, both these works use several simplifying assumptions which do not hold for a CPU multithreaded execution, for example, assumptions like (1) all the threads are synchronous, (2) execution and communication latencies are fixed and predefined, and (3) a node execution can be launched precisely in a given cycle. As such, these models cannot generate valid schedules for asynchronous multithreaded CPU execution. Hence, to the best of our knowledge, ours is the first work employing constrained optimization for multithreaded CPU scheduling of irregular DAGs.

5.4 Suggestions for future work

The two-way partitioning model in section §3.1 can be extended to P-way partitions by simply allowing the PART variable to take values in integers [0,P] instead of [0,2]. This would find P partitions of a super layer directly, avoiding recursive two-way partitioning. However, allowing values in [0,P] adds symmetries in the search space since two partitions can be switched without breaking any constraint. These symmetries prohibitively increase the run time of the solver since it keeps finding (or refuting) candidates that are just permutations of an earlier solution (or nonsolution). The usual technique of symmetry breaking using lexicographical ordering constraint on the PART variable is not sufficient because it does not break all the symmetries. A recent paper [48] proposes stricter symmetry breaking constraints for several graph optimization problems, which we believe can also be applied to this problem. We leave this as a future improvement to this work.

6 Conclusion

This paper describes GRAPHOPT, a tool developed to efficiently parallelize sparse, irregular graph workloads on parallel compute threads. Graphs are decomposed into super layers with P parallel partitions, using multiple recursions of two-way partitioning of subgraphs. The two-way partitioning problem is modeled as an optimization problem with the Minizinc constraint-modeling language and solved with the open Google OR-Tools solver. The full flow of GRAPHOPT also contains steps for workload balancing and scalability techniques to handle large graphs. The resulting performance of this super layer-based partitioning is benchmarked for sparse matrix triangular solves and sum-product networks, respectively achieving a speedup of 2.0× and 1.8× over the best existing libraries. Thus, GRAPHOPT demonstrates that constrained optimization is effective for the parallelization of large graph workloads.

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APPENDIX A

GRAPHOPT ALGORITHM

This appendix describes the different algorithms used in GRAPHOPT.

- **Algorithm 1**: The top-level algorithm of GRAPHOPT.
- **Algorithm 2**: Maps nodes to DAG layers according to the "As last as possible" (ALAP) heuristic. These DAG layers are required for the S1 scalability technique.
- **Algorithm 3**: The S1 scalability algorithm of limiting layers as described in section §3.3.
- **Algorithm 4**: The recursive two-way partitioning step M1 (section §3.1) which in turn uses the scalability techniques S2 and S3. The S2 step (section §3.3) of generating DAG components is readily available in Python’s NetworkX library.
- **Algorithm 5**: Describes the S3 step of heuristic coarsening, as explained in section §3.3.
- **Algorithm 6**: The workload balancing step explained in section §3.2.

The two-way partitioning model used in algo. 4 and 6 is described in appendix B.

---

Algorithm 1: GRAPHOPT (V_{full}, E_{full}, node\_w, nThreads)

Input: V_{full}, E_{full}: set of nodes and edges of target DAG,
node\_w: node weights,
nThreads: number of threads

Output: D_{th}: Dictionary mapping every node to a thread,
D_{sl}: Dictionary mapping every node to a superlayer

```
1 \( G_{\text{full}} \leftarrow \text{networkx.DiGraph}(V_{\text{full}}, E_{\text{full}}) \) \quad \text{▷ Graph datastructure from the NetworkX Python library}
2 \( \text{DAG\_layers} \leftarrow \text{GenDAGLayers}(G_{\text{full}}) \) \quad \text{▷ Algo 2}
3 \( V_{\text{unmapped}} \leftarrow V_{\text{full}} \)
4 \( D_{\text{th}} \leftarrow \{\} \) \quad \text{▷ Empty dictionary}
5 \( D_{\text{sl}} \leftarrow \{\} \) \quad \text{▷ Empty dictionary}
6 \text{last\_mapped\_count} \leftarrow 0 \quad \text{▷ Number of nodes mapped in the previous iteration}
7 \( sl \leftarrow 0 \) \quad \text{▷ Current superlayer index}
8
9 \textbf{while} \( V_{\text{unmapped}} \neq \emptyset \) \textbf{do}
10 \quad \( V_{\text{a}} \leftarrow \text{S1(last\_mapped\_count, } \text{DAG\_layers) } \) \quad \text{▷ Algo 3}
11
12 \quad \text{mapped\_D_{th}} \leftarrow \text{M1}_{\text{S2}_{\text{S3}}}(G_{\text{full}}, V_{\text{a}}, D_{\text{th}}, n\text{Threads}) \quad \text{▷ Algo 4}
13 \quad \text{mapped\_D_{th}} \leftarrow \text{M2}(G_{\text{full}}, \text{mapped\_D_{th}}, D_{\text{th}}, n\text{Threads}) \quad \text{▷ Algo 6}
14
15 \quad \text{curr\_V_{done}} \leftarrow \text{mapped\_D_{th}.keys()} \quad \text{▷ Dictionary keys()} are the mapped nodes
16 \quad V_{\text{unmapped}} \leftarrow V_{\text{unmapped}} \setminus \text{curr\_V_{done}}
17 \quad D_{\text{th}}.\text{update}(\text{mapped\_D_{th}})
18 \quad \text{mapped\_D_{sl}} \leftarrow \{v: sl \text{ for } v \text{ in } \text{curr\_V_{done}} \}
19 \quad D_{\text{sl}}.\text{update}(\text{mapped\_D_{sl}})
20
21 \quad \text{DAG\_layers}.\text{remove}(\text{curr\_V_{done}})
22 \quad \text{last\_mapped\_count} \leftarrow \text{len(curr\_V_{done})}
23 \quad sl++
24
25 \textbf{return} \( D_{\text{th}}, D_{\text{sl}} \)
```
Algorithm 2: GenDAGLayers \((G_{\text{full}})\)

\[\text{Generate DAG layers with "As late as possible" (ALAP) heuristic}\]

\textbf{Input:} \(G_{\text{full}}\): Full graph (in Python’s NetworkX datastructure)

\textbf{Output:} \(\text{DAG\_layers}\): Layers of DAGs in the form of list of sets of nodes

\begin{verbatim}
1 topo_order ← NetworkX.topological_sort(G_full)
2 DAG_layers ← [set() for l in range(NetworkX.dag_longest_path(G_full))]
3 for v in topo_order do
4     layer_id ← 0
5     if G_full.successors(v) then
6         layer_id ← max(layer_id of G_full.successors()) + 1
7         DAG_layers[layer_id].add(v)
8     DAG_layers.reverse()  \triangledown bottom layer at index 0
9 return DAG_layers
\end{verbatim}

Algorithm 3: S1 \((G, \text{node}_w)\)

\[\text{Limit layers (section 3.3)}\]

\textbf{Input:} \(\text{last\_mapped\_count}\): Number of nodes mapped in the last superlayer,
\(\text{DAG\_layers}\): Remaining unmapped layers

\textbf{Output:} \(V_a\): Nodes to consider for current superlayer

\begin{verbatim}
1 Va ← set()
2 for layer in DAG_layers do
3     Va ← Va ∪ layer
4     if len(Va) > α × last_mapped_count then  \triangledown Limit layers depending on the size of previous super layer. \(\alpha\) is set to 4 in our experiments
5         break
6 return Va
\end{verbatim}
Algorithm 4: M1_S2_S3 \(\langle V_a, G_{full}, node\_w, D_{th}, Y \rangle\)

\[\trianglelefteq\] Recursive two-way partitioning (section §3.1) with scalability techniques

**Input:**
- \(V_a\): Target nodes,
- \(G_{full}\): Full graph (in Python’s NetworkX datastructure),
- \(node\_w\): node weights,
- \(D_{th}\): Dictionary containing mapping of previously generated superlayers,
- \(Y\): set of target threads

**Output:** \(curr\_D_{th}\): Partitions in the form of a dictionary mapping nodes to threads

1. \(curr\_D_{th} \leftarrow \{\}\)
2. \(\text{if } \text{len}(Y) = 1 \text{ then} \quad \triangleright \text{ base case of recursion}
   3. \(th \leftarrow Y\_\text{pop()}
   4. \text{for } v \in V_a \text{ do}
   5. \quad curr\_D_{th}[v] \leftarrow th
   6. \text{return } curr\_D_{th}
7. \(subG \leftarrow G_{full}.\text{subgraph}(V_a)
8. \text{components} \leftarrow \text{NetworkX}_\text{weekly\_connected\_components}(subG) \quad \triangleright \text{S2 step}
9. \text{for } V \text{ in components do}
10. \quad \text{if } \text{len}(V) > \text{thresh}_G \text{ then} \quad \triangleright \text{Perform step S3}
11. \quad \quad currG \leftarrow G_{full}.\text{subgraph}(V)
12. \quad \quad \text{coarse}_G, \text{coarse}\_node\_w \leftarrow \text{S3}(currG, node\_w) \quad \triangleright \text{Algo 5}
13. \quad \quad V \leftarrow \text{coarse}_G.\text{nodes()}
14. \quad \quad curr\_node\_w \leftarrow \text{coarse}\_node\_w
15. \quad \text{else}
16. \quad \quad curr\_node\_w \leftarrow node\_w
17. \quad \quad nX \leftarrow \text{len}(Y) \times \text{len}(V) \big/ \text{len}(V_a)
18. \quad \quad X1 \leftarrow nX/2 \text{ threads from } Y \quad \triangleright \text{Target threads for PART}_1
19. \quad \quad Y\_\text{remove(X1)}
20. \quad \quad X2 \leftarrow nX/2 \text{ threads from } Y \quad \triangleright \text{Target threads for PART}_2
21. \quad \quad Y\_\text{remove(X2)}
22. \quad \quad \text{PART}_1, \text{PART}_2 \leftarrow \text{TwoWayPartition}(V, curr\_node\_w, X1, X2, G_{full}, D_{th}) \quad \triangleright \text{Appendix B}
23. \quad \quad \triangleright \text{If S3 (line 14) used, transform PART}_1 \text{ and PART}_2 \text{ from coarse to original nodes}
24. \quad \quad \text{curr}_D_{th\_1} \leftarrow M1_S2_S3(\text{PART}_1, G_{full}, node\_w, D_{th}, X1) \quad \triangleright \text{Recurse on each partition}
25. \quad \quad \text{curr}_D_{th\_2} \leftarrow M1_S2_S3(\text{PART}_2, G_{full}, node\_w, D_{th}, X2)
26. \quad \quad \text{curr}_D_{th\_update}(\text{curr}_D_{th\_1})
27. \quad \quad \text{curr}_D_{th\_update}(\text{curr}_D_{th\_2})
28. \text{return } curr\_D_{th}
Algorithm 5: S3 \((G, \text{node}_w)\)

\[\texttt{Heuristic coarsening (section 3.3)}\]

\textbf{Input}: \(G\): Target graph (in Python's NetworkX datastructure),
\(\text{node}_w\): node weights,

\textbf{Output}: \(\text{coarse}_G\): Coarse graph,
\(\text{coarse}_w\): coarse node weights,

\begin{enumerate}
\item \(\text{root}_\text{nodes} \leftarrow \text{nodes in } G \text{ with no successors}\)
\item \(\text{done}_\text{nodes} \leftarrow \emptyset\)
\item \(\text{depth}_\text{diff} \leftarrow 0\)
\item \(\text{depth}_\text{diff}_\text{ls} \leftarrow \emptyset\)
\item \(\text{dfs}_\text{node}_\text{ls} \leftarrow \emptyset\)
\end{enumerate}

\begin{enumerate}[a)]
\item \(\text{while } \text{root}_\text{nodes} \text{ do}\)
\item \(\text{stack} \leftarrow [\text{root}_\text{nodes}.\text{pop()}]\)
\item \(\text{while } \text{stack} \text{ do}\)
\item \(\text{curr}_v \leftarrow \text{stack}[-1]\) \hspace{1em} \text{Last element from the stack}
\item \(\text{depth}_\text{diff} ++\)
\item \(\text{next}_\text{ls} \leftarrow [v | v \in G.\text{predecessors}(\text{curr}_v) \text{ and } v \notin \text{done}_\text{nodes}]\)
\item \(\text{if } \text{next}_\text{ls} \text{ then}\)
\item \(\quad \text{stack}.\text{extend}(\text{next}_\text{ls})\)
\item \(\text{else}\)
\item \(\quad \text{done}_\text{nodes}.\text{add}(\text{curr}_v)\)
\item \(\quad \text{node}_\text{ls}.\text{append}(\text{curr}_v)\)
\item \(\quad \text{depth}_\text{diff}_\text{ls}.\text{append}(\text{depth}_\text{diff})\)
\item \(\quad \text{depth}_\text{diff} \leftarrow 0\)
\item \(\quad \text{stack}.\text{pop()}\) \hspace{1em} \text{Pop } \text{curr}_v \text{ from the stack}
\end{enumerate}

\begin{enumerate}[a)]
\item \(\text{Generate coarse nodes}\)
\item \(\text{map}_\text{coarse}_\text{node}_\text{to}_\text{node}_\text{set} \leftarrow \{}\)
\item \(\text{coarse}_w \leftarrow \{}\)
\item \(\text{coarse}_\text{nodes}_\text{id} \leftarrow 0\)
\item \(\text{curr}_\text{node}_\text{set} \leftarrow \emptyset\)
\item \(\text{curr}_w \leftarrow 0\)
\item \(\text{size}_\text{threshold} \leftarrow \frac{G.\text{size}()}{1000}\) \hspace{1em} \text{coarse}_G \text{ will have around 1000 coarse nodes}
\item \(\text{depth}_\text{threshold} \leftarrow \log(\text{size}_\text{threshold})\)
\item \(\text{degree}_\text{threshold} \leftarrow 10\)
\item \(\text{for } (i, v) \text{ in enumerate}(\text{dfs}_\text{node}_\text{ls}) \text{ do}\)
\item \(\quad \text{if } (\text{len}(\text{curr}_\text{node}_\text{set}) > \text{size}_\text{threshold}) \text{ or}\)
\item \(\quad\quad (\text{depth}_\text{diff}_\text{ls}[i] > \text{depth}_\text{threshold}) \text{ or}\)
\item \(\quad\quad (G.\text{out}\_\text{degree}(v) > \text{degree}_\text{threshold}) \text{ then}\) \hspace{1em} \text{Create a coarse node}
\item \(\quad \text{map}_\text{coarse}_\text{node}_\text{to}_\text{node}_\text{set}[\text{coarse}_\text{node}_\text{id}] \leftarrow \text{curr}_\text{node}_\text{set}\)
\item \(\quad \text{curr}_\text{node}_\text{set}.\text{set}()\)
\item \(\quad \text{coarse}_w[\text{coarse}_\text{node}_\text{id}] \leftarrow \text{curr}_w\)
\item \(\quad \text{curr}_w \leftarrow 0\)
\item \(\quad \text{coarse}_\text{node}_\text{id}++\)
\item \(\quad \text{curr}_\text{node}_\text{set}.\text{add}(v)\)
\item \(\quad \text{curr}_w += \text{node}_w[v]\)
\end{enumerate}

\begin{enumerate}[a)]
\item \(\text{coarse}_G \leftarrow \text{Generate python NetworkX graph from } \text{map}_\text{coarse}_\text{node}_\text{to}_\text{node}_\text{set} \text{ and } G\)
\item \(\text{return } \text{coarse}_G, \text{coarse}_w\)
\end{enumerate}
Algorithm 6: M2 \( (G_{\text{full}}, \text{node}_w, \text{imbalanced}_D_{\text{th}}, D_{\text{th}}, n\text{Threads}) \)

\[ \triangle \text{Balance partitions (section \S3.2)} \]

**Input:**
\( G_{\text{full}} \): Full graph (in Python’s NetworkX datastructure),
\( \text{node}_w \): node weights,
\( \text{imbalanced}_D_{\text{th}} \): Imbalanced partitions, represented as a dictionary mapping nodes to threads,
\( D_{\text{th}} \): Dictionary containing mapping of previously generated superlayers,
\( n\text{Threads} \): number of threads

**Output:**
\( \text{balanced}_D_{\text{th}} \): Balanced partitions, represented as a dictionary mapping nodes to threads

1. \( \text{partition}_ls \leftarrow [\{ v \mid \text{imbalanced}_D_{\text{th}}[v] = \text{th} \} \mid \forall \text{th} \in [0, n\text{Threads})] \) \( \triangle \) list of partitions (which are represented as sets)
2. \( \text{thread}_pool \leftarrow n\text{Threads} \)
3. \textbf{while} \( \text{len(thread}_\text{pool}) > 1 \) \textbf{do}
4. \( \text{th}_L \leftarrow \text{Thread with largest partition among thread}_\text{pool} \)
5. \( \text{th}_S \leftarrow \text{Thread with smallest partition among thread}_\text{pool} \)
6. \( L \leftarrow \text{partition}_ls[\text{th}_L] \) \( \triangle \) currently largest partition
7. \( S \leftarrow \text{partition}_ls[\text{th}_S] \) \( \triangle \) currently smallest partition
8. \( \text{Combined} \leftarrow S \cup L \)
9. \( L', S' \leftarrow \text{TwoWayPartition} (\text{Combined}, \text{node}_w, \{\text{th}_L\}, \{\text{th}_S\}, G_{\text{full}}, D_{\text{th}}) \) \( \text{\( \triangle \) Appendix B} \)
10. \textbf{if} \( \min(\text{len}(L'), \text{len}(S')) > \text{len}(S) \) \textbf{then} \( \triangle \) New partitions are more balanced
11. \( \text{partition}_ls[\text{th}_L] \leftarrow L' \)
12. \( \text{partition}_ls[\text{th}_S] \leftarrow S' \)
13. \textbf{else} \( \triangle \) L is not divisible further due to lack of parallelism. Do not try again.
14. \( \text{thread}_\text{pool}.\text{remove}(L) \)
15. \textbf{for} \( (\text{th}, \text{partition}) \) in enumerate(\( \text{partition}_ls \)) \textbf{do}
16. \textbf{for} \( v \) in \( \text{partition} \) \textbf{do}
17. \( \text{balanced}_D_{\text{th}}[v] \leftarrow \text{th} \)
18. \textbf{return} \( \text{balanced}_D_{\text{th}} \)
APPENDIX B

TWO-WAY PARTITIONING MODEL

The code listing 1 is the minizinc-based optimization model for two-way partitioning of graphs, as described in section §3.1. A python wrapper to this minizinc model generates the input parameters like \(V_{in}, E_{in}, PART_{in}\) from the graph structure and mapping of previous superlayers. The code listing 2 describes the input parameters to the model for the example shown in fig. 6.

```plaintext
1 %%% input parameters %%%
2 int: n_V; % number of nodes in graph \(G\)
3 set of int: V = 1..n_V;
4 int: max_node_w; % maximum node weight in current \(G\)
5 array[V] of 1..max_node_w: node_w;
6 int: n_E;
7 array[1..n_E, 1..2] of int: E; % edges (an array (instead of a set) of tuples, for ease of modelling)
8 int: n_Vin;
9 set of int: Vin = 1..n_Vin; % source nodes on incoming edges
10 int: n_Ein;
11 array[1..n_Ein, 1..2] of int: Ein;
12 array[Vin] of 1..2: PARTin;

13 %%% decision variables %%%
14 array[V] of var 0..2: PART;
15 var 0..(max_node_w * n_V): PART_1_size;
16 var 0..(max_node_w * n_V): PART_2_size;
17 array[1..n_Ein] of var bool: Ein_crossings;

18 %%% constraints %%%
19 % acyclic and data-dependency constraint
20 constraint forall (e in 1..n_E) {
21   let {
22     int : src = E [e, 1]; % local variables for readability
23     int : dst = E [e, 2];
24   } in
25   PART [dst] = PART [src] \/
26   PART [dst] = 0
27);
28
29 % partition sizes constraint
30 constraint PART_1_size = sum ( [ node_w[v] | v in V where PART[v] == 1 ] );
31 constraint PART_2_size = sum ( [ node_w[v] | v in V where PART[v] == 2 ] );
32
33 % inter-thread communication constraint
34 constraint forall (e in 1..n_Ein) {
35   let {
36     int : src = Ein [e, 1]; % local variables for readability
37     int : dst = Ein [e, 2];
38   } in
39   Ein_crossings [e] =
40   ( PART [dst] != 0 \/
41     PART [dst] != PARTin [src]
42   )
43 };
44
45 %%% objective %%%
46 solve maximize 10 * min (PART_1_size, PART_2_size) - sum (Ein_crossings);
```

Listing 1. Minizinc code for the two-way partitioning optimization model described in section §3.1
Listing 2. Parameters for the example in fig. 6 to be passed as inputs to the model in listing 1