NeutronTask: Scalable and Efficient Multi-GPU GNN Training with Task Parallelism

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ABSTRACT

Graph neural network (GNN) training requires extensive memory and computational resources. Thus, researchers propose multi-GPU processing, partitioning graph data across GPUs for parallel training. However, vertex dependencies cause significant neighbor replication across GPUs, increasing memory usage. Additionally, the intermediate data generated during training further exacerbates memory consumption, with neighbor replication and intermediate data typically accounting for over 80% of the total memory usage.

In this paper, we propose task parallelism for multi-GPU GNN training, which reduces neighbor replication by partitioning tasks in each layer across GPUs, instead of the graph structure. This approach only partitions graph data within GPUs, reducing memory usage of each task and overlapping subgraph computation across GPUs. Shared neighbor embeddings among different subgraphs can be efficiently reused within a single GPU. Additionally, we employ a task-decoupled GNN training framework, which decouples different training tasks to release their intermediate data in advance. By integrating these techniques, we propose a multi-GPU GNN training system, NeutronTask. Experimental results on a 4×A5000 GPU server show that NeutronTask effectively supports billion-scale full-graph GNN training. For small graphs, NeutronTask achieves $1.27\times - 5.47\times$ speedup compared to state-of-the-art GNN systems.

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Table 1: Memory consumption of graph topology (Topo), feature (Feat), model parameters (Params), and intermediate data (Intr) for a 3-layer GCN training.

Dataset	#hidden	Params	Topo	Feat	Intr
ogbn-products	256	0.4MB	0.24GB	0.9GB	10.68GB
ogbn-papers100M	128	0.25MB	6.4GB	52.97GB	335.95GB

PVLDB Artifact Availability:
The source code, data, and/or other artifacts have been made available at https://github.com/iDC-NEU/NeutronTask.

1 INTRODUCTION

Graph Neural Networks (GNNs) have demonstrated superior performance across various practical applications such as social networks [29, 68, 75], recommendation systems [15, 67, 74], financial fraud detection [61], protein structure analysis [18], drug prediction [37, 49], traffic forecasting [6, 28], and natural language processing [42, 73]. GNN training consists of two tasks in each model layer: **embedding transformation** (T) and **graph propagation** (P). Each vertex applies T to update vertex embeddings and uses P to propagate neighbor embeddings. By iteratively executing these two tasks, GNN can learn rich structural information of data samples.

Recently, full-graph GNN training has emerged as a promising GNN training method as it provides more stable model quality compared to mini-batch training [27, 52, 55, 60, 63–65, 77]. However, full-graph GNN training requires extensive memory and computational resources [60, 63]. Considering the continuously increasing size of real-world graphs, researchers have proposed employing multi-GPU processing to meet the resource-intensive requirements of large-scale GNN training [8, 9, 19, 27, 43, 54, 65, 71]. These systems typically employ data parallelism, partitioning the input graph to enable parallel computation across multiple GPUs and handle remote neighbor aggregation by caching neighbor replicas. Despite the significant performance improvements achieved by multi-GPU processing, handling large-scale graphs remains a challenge due to the substantial disparity between the limited memory capacity of GPUs and the extensive memory consumption. As shown in Figure 1(a), this memory consumption primarily comes from neighbor

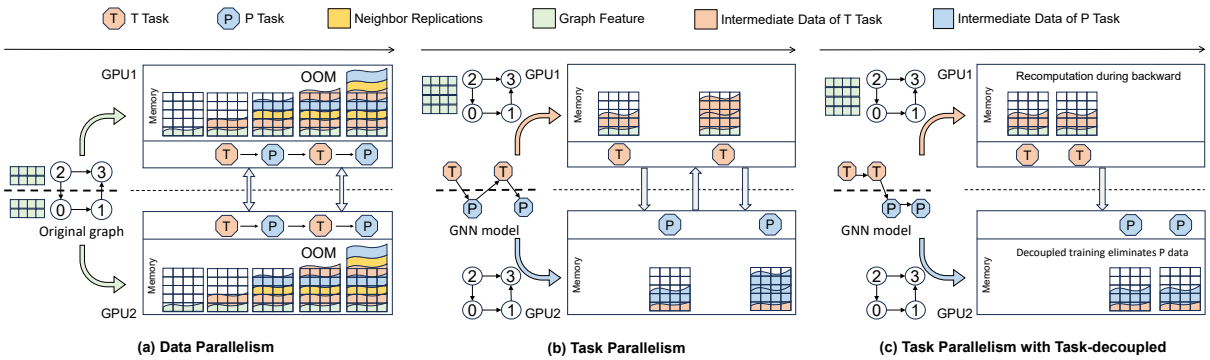

Figure 1: GNN data parallelism vs. GNN task parallelism. The square matrix inside the GPU represents GPU memory space, and The arrows between GPUs represent communication. (a) GNN data parallelism requires caching neighbor replications and intermediate data to complete backward propagation, leading to out-of-memory (OOM) errors. (b) GNN task parallelism partitions training tasks across GPUs rather than partitioning the graph, reducing neighbor replications. (c) GNN task parallelism with task-decoupled breaks the alternated execution of the T and P tasks, releasing the intermediate data of P tasks in advance.

replication (in yellow) and intermediate data (in orange and blue), accumulating with the increasing number of GNN tasks.

The neighbor replication arises from inter-GPU graph partition in data parallelism. When an entire graph is partitioned across multiple GPUs, the common neighbors between subgraphs must be stored multiple times on different GPUs. The neighbor replication increases rapidly with the number of graph partitions. Taking the ogbn-papers100M dataset as an example, when the number of partitions reaches 8, the size of neighbor replication increases by 200.1GB. Since each model layer requires additional memory to cache neighbor embeddings, the memory consumption associated with neighbor replication increases with the deeper model layers.

The intermediate data includes the vertex embeddings of various tasks [63]. During forward propagation, each model layer generates vertex embeddings, which are cached and consumed in the gradient computation of each layer during backward propagation. In GNN models, T tasks and P tasks are executed alternately. Although the linear P task is not directly involved in parameter updates, the input of T is the output of P, and the output of P is required when calculating the gradient of the parameter in T. Therefore, the vertex embeddings of T tasks and P tasks both need to be cached. We conduct experiments using NeutronStar [64] in a single-CPU environment to evaluate the memory consumption of intermediate data. As shown in Table 1, for a 3-layer GCN training, the intermediate data averages 86.38% of total memory usage.

In this paper, we reduce the memory consumption caused by neighbor replication and intermediate data through two key techniques. Firstly, we propose task parallelism for GNN training to reduce neighbor replications through inter-GPU task partition and intra-GPU graph partition. As illustrated in Figure 1(b), GNN task parallelism partitions T and P tasks in each model layer across different GPUs, such that each GPU only needs to handle one type of task. Intra-GPU graph partition splits each training task over the entire graph into smaller processing units (subgraphs), ensuring each task can be sequentially scheduled on a single GPU, without exhausting the GPU memory. Concurrently, the subgraph computation can be overlapped across different GPUs to enhance parallelism. The shared neighbor embeddings among different subgraphs can be efficiently reused within a single GPU. As a result, GNN task parallelism effectively reduces neighbor replication by avoiding inter-GPU graph partition. Secondly, we propose a task-decoupled GNN training framework to reduce the memory consumption of intermediate data. The framework transforms the alternating execution mode of T tasks and P tasks into a sequence where continuous P tasks follow continuous T tasks. As illustrated in Figure 1(c), this approach not only reduces intermediate data generated by linear P tasks but also facilitates the use of traditional DNN recomputation techniques [12] to reduce the runtime memory consumption of intermediate data. In addition, the framework offers a flexible task scheduling model that allocates different numbers of GPUs to P and T tasks to meet the different resource requirements of P and T tasks. By integrating the above techniques, we propose a multi-GPU system for full-graph GNN training, NeutronTask. The experimental results on a 4-GPU (A5000) server demonstrate that NeutronTask can train large-scale graphs and achieve performance improvements compared to Sancus [43] and NeutronStar [64].

Our primary contributions are summarized as follows:

- We propose GNN task parallelism, which reduces neighbor replication by partitioning tasks across GPUs and partitioning graph of each task within a GPU, instead of partitioning graph data across GPUs.
- We propose a task-decoupled GNN framework that decouples T and P tasks. Then, we utilize the recomputation technique and flexible resource allocation to improve memory efficiency.
- We develop NeutronTask, a multi-GPU accelerated system that reduces memory usage by $49\% - 67\%$ and achieves $1.27\times - 5.47\times$ speedup compared to the state-of-the-art GNN training system.

The rest of this paper is summarized as follows. Section 2 introduces the background information of this work. Section 3 gives an overview of NeutronTask. Section 4 provides a detailed description of GNN task parallelism. Section 5 introduces the task-decoupled GNN training framework, including the task-decoupled training and task scheduling model. Section 6 analyzes the experimental results. Section 7 discusses the limitations and future work. Section 8 discusses related work. Section 9 summarizes the paper.

2 PRELIMINARIES

2.1 Graph Neural Network

Graph data are utilized to manage real-world data due to their ability to express entities and their relationships efficiently [3, 14, 20–22, 36, 39, 57]. As input to GNNs, graph data can be represented as $G =$

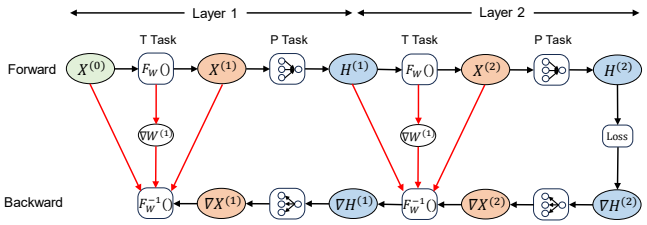

Figure 2: The data flow of a 2-layer GCN. The ellipses represent vertex embeddings at different stages, which need to be cached in the GPU memory. The red arrows connect to the dependent data, representing parameter gradient computations in backward propagation.

(V, E), where V and E represent vertex and edge sets, respectively, and each vertex contains a feature vector X_v, where $(v \in V)$.

GNN Models. GNN models consist of multiple layers, which generate embeddings by leveraging the structural and feature information of the graphs. Each layer of the GNN model consists of T and P tasks. T tasks apply neural networks to extract the information of vertices or edges, generating updated embeddings. P tasks include scattering vertex embeddings to edges or neighbors. We formalize these tasks using the aggregate-update computation pattern:

$$X_v^{(l)} = UPDATE(X_v^{(l-1)}, W^{(l)}), \quad (1)$$

$$H_v^{(l)} = AGGREGATE(\{X_u^{(l)} | \forall u \in N_{in}(v)\}), \quad (2)$$

where $X_v^{(l-1)}$ and X_v^l represents the embedding of vertex v in the $(l-1)$-th layer and l-th layer respectively. $X_v^{(0)}$ represents the input feature of vertex v. $N_{in}(v)$ represents the incoming neighbors of vertex v. Model parameters exist only in T tasks, while P tasks are responsible solely for propagating and aggregating vertex information. The model parameters are updated through gradient computation during the backward propagation.

Different GNN models are characterized by different functions of $UPDATE$ and $AGGREGATE$. For instance, GCN [29] aggregates neighbors by the Symmetric Normalized Laplacian in P tasks and uses neural networks to update vertex embeddings in T tasks. The formula for a single-layer GCN is as follows:

$$H^{(l+1)} = \sigma\left(\tilde{D}^{-\frac{1}{2}}\tilde{A}\tilde{D}^{-\frac{1}{2}}W^{(l)}\right), \quad (3)$$

where σ represents the activation function, $W^{(l)}$ represents the neural network parameter of the l-th layer. The $\tilde{A}$ and $\tilde{D}$ correspond to $A + I$ and $D + I$, where A represents the adjacency matrix, D represents the degree matrix and $D_{ii} = \sum^j A^{ij}$.

Intermediate Data in GNN Training. Intermediate data in full-graph GNN training refers to the inputs and outputs of T and P tasks for each GNN layer, which is generated during the forward propagation and cached to compute gradients for T tasks during backward propagation [63]. Figure 2 is the data flow in a 2-layer GCN [29] model. In forward propagation, each vertex updates its embedding to generate updated results (*i.e.,* $X^{(i)}$) by the T task, which generates intermediate data of the neural network model for gradient computation. Then, each vertex aggregates neighbors' embeddings to generate aggregation results (*i.e.,* $H^{(i)}$). Both neighbor embeddings and aggregated results need to be cached. The final layer's vertex embeddings (*i.e.,* $H^{(2)}$) compute the loss value based on truth data labels, generating gradient vectors (*i.e.,* $\nabla H^{(2)}$), whose dimensions match those of the vertex embeddings. Backward propagation starts from the final layer to the first, computing model parameter gradients using vertex gradients and embeddings. Each layer applies the chain rule for vertex gradient computation, including gradient propagation and derivative computation. Intermediate data from forward propagation must be retained until gradient computation for the corresponding backward layer is completed.

Table 2: Neighbor replication factor (α) and total memory consumption (MC) in the ogbn-papers100M dataset under varying numbers of partitions (3-layer GCN).

Partitions	1	2	4	8	16	32	64
NR	1	1.25	1.52	2.13	3.02	4.46	6.34
MC (/GB)	335.95	380.22	428.03	536.05	693.65	948.65	1281.56

2.2 Multi-GPU GNN Systems with Data Parallelism

Given the resource-intensive requirement of large-scale GNN training, researchers have employed multi-GPU processing to accelerate the training process. As shown in Figure 3, a common approach to scaling GNN training across multiple GPUs is data parallelism, which partitions the graph data across multiple GPUs to enable parallel training. During GNN training, P tasks may require access to neighbor vertices located on remote GPUs, leading to substantial vertex dependencies (the dashed vertices in Figure 3). To manage these dependencies, GNN data parallelism involves inter-GPU communication to fetch remote vertex data, followed by creating local replicas of these remote vertices to facilitate local computation.

Neighbor replication refers to each GPU creating replicas of neighbors from remote GPUs, which increases memory consumption. We evaluate the memory consumption of neighbor replication in the ogbn-papers100M dataset under varying numbers of partitions. We quantify the size of neighbor replication using the replication factor α, defined as the average number of replicas per vertex. The results are presented in Table 2, where the scale of neighbor replication rises rapidly with the number of partitions. As the number of partitions expands from 1 to 64, neighbor replication causes the total memory consumption to increase by 3.81×.

Despite multi-GPU platforms offering increased memory availability, the substantial volume of neighbor replication and intermediate data still hinders the effectiveness and efficiency of GNN data parallelism in handling large-scale GNN training. For real-world graphs, the data often exceeds the memory capacity even with multiple GPUs. As shown in Table 2, training a 3-layer GCN model on the ogbn-papers100M dataset requires at least 428.03GB of available memory when the number of partitions is 4. Even with 4 NVIDIA A100 GPUs (each with 80GB), there remains a discrepancy between the available and required memory. Some recent works [27, 64] propose offloading data storage to the CPU to alleviate GPU memory consumption. However, these frameworks introduce frequent data switches between the CPU and GPU. Given the low-bandwidth PCIe connection between the CPU and GPU, such frequent data transfers can significantly impact performance [63].

In summary, the performance and scalability of existing frameworks are still limited by the substantial neighbor replication across multiple GPUs. Avoiding the partitioning of graph data across different GPUs is crucial to addressing these issues. In this paper, we explore task parallelism approaches for multi-GPU GNN training by fully partitioning GNN tasks before partitioning the graph

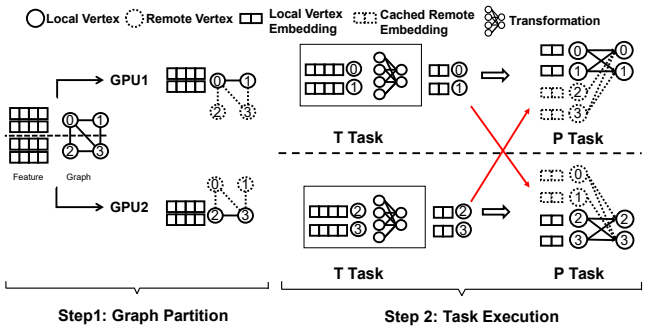

Figure 3: The data parallelism training flow for a single-layer GNN and the generation of neighbor replications.

structure. This strategy minimizes graph partitions and reduces communication and memory overhead from neighbor replication.

3 THE NEUTRONTASK

We propose NeutronTask, a multi-GPU system for large-scale GNN training, which reduces memory consumption caused by neighbor replication and intermediate data through two key techniques. Figure 4 provides an architecture overview of NeutronTask.

GNN Task Parallelism. NeutronTask designs GNN task parallelism, which reduces the substantial memory consumption caused by neighbor replication in GNN data parallelism. Firstly, we partition the T and P tasks of each model layer across different GPUs. This ensures that the memory consumption of each GPU is limited to the intermediate data generated by the allocated tasks, rather than managing all tasks and neighbor replications as in data parallelism. Secondly, we employ the intra-GPU graph partition to address the issue where the memory requirements of a single training task exceed the GPU memory. Then, we design a vertex dependency management approach with cross-subgraph neighbor reusing and random subgraph grouping, caching neighbors on the same GPU to prevent replication. Additionally, the subgraph computation and communication can be overlapped to improve performance. Thirdly, we propose a hybrid parallelism approach to efficiently utilize scenarios where the number of GPUs exceeds the number of tasks. By adopting these strategies, GNN task parallelism significantly enhances the scalability and efficiency of multi-GPU GNN training.

Task-decoupled GNN Training Framework. Full-graph GNN training caches large intermediate data, which can only be released during backward propagation. The linear P tasks do not contain parameters, and caching its intermediate data is caused by the alternating execution of T and P tasks. To address this, we propose a task-decoupled GNN training framework, which extends the decoupled training to task parallelism. Specifically, we separate T and P tasks within the GNN model, executing all T tasks first, followed by all P tasks. This framework reduces intermediate data from P tasks and facilitates using traditional DNN recomputation techniques [12] to reduce intermediate data from T tasks. Additionally, we provide a flexible task scheduling model, which adjusts the number of GPUs executing T and P tasks and meets different resource requirements to enhance training performance.

4 GNN TASK PARALLELISM

In this section, we provide a detailed design of GNN task parallelism, including task partition and intra-GPU graph partition.

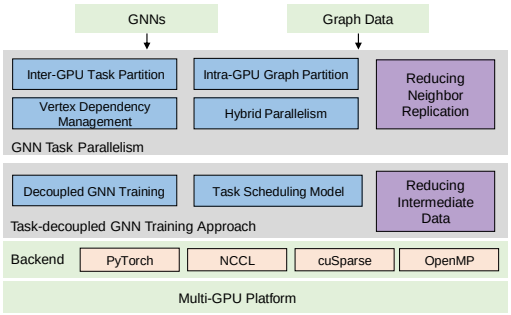

Figure 4: NeutronTask overview.

4.1 Task Partition

Based on the following observations, we propose partitioning tasks across GPUs rather than partitioning the graphs. Firstly, T and P tasks have distinct computational characteristics and resource requirements. T tasks involve contiguous storage and matrix multiplication of vertex embeddings and model parameters, making them compute-intensive. P tasks involve frequent random memory access, making them memory-intensive. Therefore, partitioning tasks on the same GPU leads to significant memory requirements and prevents full utilization of GPUs. In contrast, partitioning tasks across GPUs allows for tailored optimizations based on the specific computational and memory characteristics of T and P tasks, ultimately improving performance. Secondly, the intermediate data generated by T and P tasks serve different roles. Storing them separately has no impact on model training. The intermediate data of T tasks is to compute neural network parameter gradients, which is the main objective of GNN training. The intermediate data of P tasks is used to link the computation graphs between two T tasks.

Initial Partitioning Setting. Based on the above analysis, we partition the T and P tasks of each model layer across different GPUs. This requires coordinating the allocation by considering the relationship between the number of GPUs and tasks. Based on the number of GPUs (N_{GPU}) and GNN tasks (N_{task}) are determined, we provide three initial partitioning strategies:

- **When** $N_{GPU} < N_{task}$**:** We allocate the same type of tasks to the same GPU, so each GPU handles only one computational characteristic (either compute-intensive or memory-intensive), maximizing resource utilization.
- **When** $N_{GPU} = N_{task}$**:** Each GPU executes a single task, reducing memory requirement by avoiding neighbor replication.
- **When** $N_{GPU} > N_{task}$**:** We use a hybrid parallelism approach, grouping GPUs to use data parallelism within groups and task parallelism between groups. The neighbor replication occurs only within P task groups.

4.2 Intra-GPU Graph Partition

GNN task parallelism execution flow is illustrated in Figure 5(a), where four GPUs are responsible for T tasks and P tasks in each model layer, respectively. Initially, the entire graph data is processed by GPU1 for the T tasks, and the results are then transferred to GPU2 for the P tasks. We propose an intra-GPU graph partition to address situations where the intermediate data generated by the allocated tasks exceeds a single GPU memory capacity and to overlap the computation of GPUs. All GPUs use the same partitioning strategy to partition the entire graph into multiple subgraphs that fit within a single GPU memory and then process them sequentially.

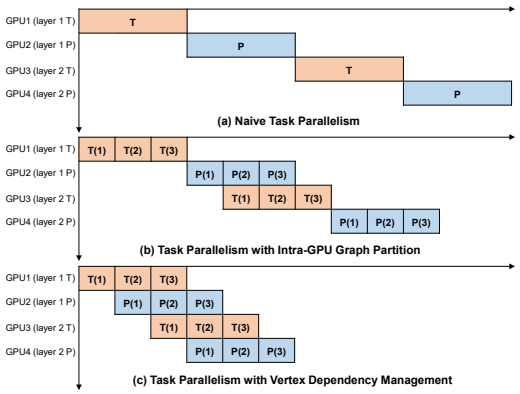

Figure 5: GNN task parallelism with intra-GPU graph partition on the forward propagation of a 2-layer GNN model. (i) represents the i-th subgraph.

With intra-GPU graph partition, the training flow of GNN task parallelism is illustrated in Figure 5(b). The input graph is partitioned into three subgraphs, each storing a disjoint set of vertices along with their vertex dependencies. Vertex dependencies necessitate that the P tasks of each subgraph involve vertex embeddings from other subgraphs in their computations. For instance, GPU2 cannot execute the P task for subgraph 1 until the T task of all subgraphs in GPU1 has been completed.

Vertex Dependency Management Approach. To reduce the waiting time of GPUs executing P tasks and enable the task-level pipeline parallelism illustrated in Figure 5(c), we design a vertex dependency management approach. Firstly, cross-subgraph neighbors located within the same GPU can be reused. As illustrated in Figure 5(b), after GPU2 executes the P tasks for subgraph 1, it caches the neighbors that belong to subgraph 2 and subgraph 3. When subgraph 2 and subgraph 3 are executed, these neighbors can be reused. Since these neighbors are cached only once within GPU2, it avoids neighbor replication. Secondly, to overlap the computation between subgraphs as shown in Figure 5(c), we apply an approach similar to ClusterGCN [13], which skips the aggregation of uncomputed neighbor embeddings and reconfigures the edges within each subgraph at the beginning of every epoch to ensure that all neighbors are computed. As shown in Figure 6, we divide the entire graph into multiple chunks, where $C[i][j]$ represents the graph structure with destination vertices in chunk i and source vertices in chunk j. Before the start of each epoch, multiple chunks are randomly regrouped into a subgraph, allowing the edges between these chunks to be trained in the current epoch. From a probabilistic perspective, as the number of training epochs increases, different chunks have a chance to combine into one subgraph, meaning all edges have a probability of being computed.

Algorithm 1 outlines the flow for executing the P task using vertex dependency management. To begin with, we initialize the aggregated vertex embeddings to zero (line 1). Then, we shuffle the chunks and group every k chunks into a subgraph (*i.e.,* $k = \frac{M}{S}$) (line 3). In the task executing stage, we traverse each subgraph s, with chunk $i \in [s{*}k, (s{+}1){*}k]$ belonging to the current subgraph (lines 5-21). For the chunks before subgraph s, we reuse the cached neighbor embeddings for aggregation (lines 10-13), while the chunks after s will be dropped. It is worth mentioning that we utilized sparse matrix multiplication with cuSparse to execute P tasks, which is suitable for leveraging the CPU capability. After completing the aggregation computation within each chunk of a subgraph, we cache the subset of vertices that have dependencies on chunks following the subgraph s (line 19). Finally, we return the aggregated vertex embeddings of the P task (line 22).

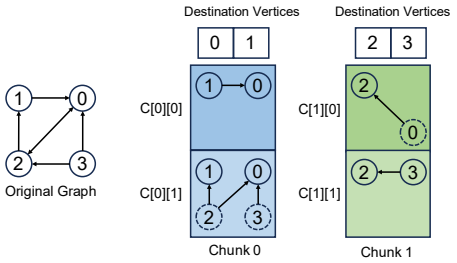

Figure 6: Chunk-based graph structure.

Algorithm 1 The P tasks using vertex dependency management.

Input: Graph chunks $C[i][j]$, The number of chunks M, The number of subgraphs S, Vertex embeddings of each chunk i X_i
Output: Aggregated vertex embeddings: $H_0, H_1, \cdots, H_M$

```
1:  Init H_0, H_1, ..., H_M;
2:  // Every k chunks will be grouped into a subgraph (k = M/S)
3:  k, C' = Chunk_Shuffle(C, M, S);
4:  // Traverse each subgraph
5:  for s ← 0, ..., S − 1 do
6:      // Traverse all chunks within this subgraph
7:      for i ← s ∗ k, ..., (s + 1) ∗ k do
8:          // Traverse all chunks prior to this subgraph
9:          for j ← 0, ..., (s + 1) ∗ k do
10:             if j < s ∗ k then
11:                 //Reuse the embeddings of computed subgraphs
12:                 X = load({X_j | ∀j ∈ C'[i][j]});
13:                 h = AGG_with_reuse(X);
14:             else
15:                 h = AGG({X_j} | ∀j ∈ C'[i][j]});
16:             end if
17:             H_i.add(h);
18:         end for
19:         Caching X_i;
20:     end for
21: end for
22: return H_0, H_1, ..., H_M;
```

The Effectiveness of Task Parallelism. For data parallelism, the boundary vertices of each subgraph (B_i) may be replicated on other GPUs and each GPU caches the embeddings of the remote neighbors and local vertices. Assuming the average replication count is β, where $1 < \beta \leq (M-1)$, the memory requirement for P tasks can be formalized as $MR_{dp} = \sum_i^M (\beta \cdot |B_i| + |V_i|) \cdot L \cdot |d|$, where M represents the number of GPUs, L represents the model layers, and $|d|$ represents the average dimension of hidden layers. For task parallelism, each subgraph is loaded onto each GPU sequentially, and the memory requirement for P tasks is $MR_{tp} = \sum_{i=1}^M (|B_i| + |V_i|) \cdot L \cdot |d|$. Since $\beta > 1$, we have $MR_{tp} < MR_{dp}$. Therefore, task parallelism has lower memory requirements than data parallelism.

4.3 Hybrid Parallelism

We propose hybrid parallelism to address the scenario where the number of GPUs exceeds the number of GNN tasks. Hybrid parallelism combines data parallelism and task parallelism through a

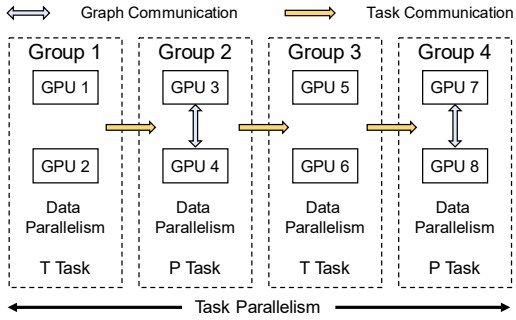

Figure 7: An illustration of hybrid parallelism.

grouping mechanism, with data parallelism within groups and task parallelism between groups. This approach maximizes resource utilization on multi-GPU platforms while minimizing neighbor replication compared to solely data parallelism.

The grouping mechanism is illustrated in Figure 7. All GPUs are divided into groups according to the number of tasks, with each group handling one task. Within each group, data parallelism is used. Taking the ogbn-papers100M from Table 2 as an example, the issue in Figure 7 causes only 1.25× neighbor replication. Compared to data parallelism with 8 GPUs (2.13×), hybrid parallelism reduces neighbor replications by 1.7×. This is because only the group handling the P task generates neighbor replications. Consequently, hybrid parallelism reduces neighbor replication by minimizing graph partitions, making it advantageous for training large-scale graphs.

Hybrid parallelism executes task parallelism between groups. The chunk-based graph structure shown in Figure 6 can be directly applied to hybrid parallelism. Specifically, we set the chunk count as a multiple of GPUs in a group, ensuring each GPU processes an equal share for workload balance. It is worth mentioning that if each group consists of a single GPU, hybrid parallelism degrades into GNN task parallelism. In summary, hybrid parallelism is utilized when there are a large number of GPUs. The core idea is to use idle GPUs to help heavily workload GPUs complete training tasks.

5 TASK-DECOUPLED GNN TRAINING FRAMEWORK

In this section, we extend the decoupled GNN training to NeutronTask by a task-decoupled approach, reducing the intermediate data of P tasks and naturally utilizing recomputation techniques to release the intermediate data of T tasks early. Then, we design a task scheduling model that adjusts the number of GPUs allocated to T and P tasks to combine the task-decoupled approach with GNN task parallelism. Finally, we give the overall workflow of NeutronTask.

5.1 Task-decoupled GNN Training

Decoupled GNN Techniques. Related studies [25, 66] show that the character with T tasks extracting feature information and P tasks learning structural information drives the efficiency of GNNs, rather than alternating execution mode. Therefore, some decoupled GNN models [11, 24, 30, 35, 48, 50, 66, 81, 83] advocate separating the execution of T and P tasks, achieving high model accuracy and scalability. A recent work (NeutronTP) [2] has extended decoupled GNN training to general GNN training , reducing the frequency of distributed communication caused by tensor parallelism while providing convergence proof to ensure model accuracy. Specifically, the general decoupled GNN training is as follows:

$$Y = g_\theta(X^{(0)}) \cdot e_\theta\big(g_\theta(X^{(0)}), A\big) \cdot f(\hat{A}), \tag{4}$$

where $g_\theta()$ represents vertex-based T tasks, transforming the input features into vertex embeddings. $e_\theta()$ represents the Scatter P task and edge-based T task, which send vertex embeddings to edges to compute edge weights. $f()$ represents P tasks, which perform multi-layer graph propagation using edge weight.

Task-decoupled Approach. In this paper, we further analyze the role of decoupled training techniques in reducing memory requirements during GNN training. We integrate GNN task parallelism with the decoupled training and propose a task-decoupled approach that immediately releases the intermediate data generated by P tasks. As shown in Figure 8(b), the P tasks are extracted from the GNN model and executed consecutively after all T tasks. During backward propagation, consecutive P tasks only need to propagate and aggregate vertex gradients, and their intermediate data does not need to be stored (*i.e.,* $H^{(i+1)}$ and $H^{(i+2)}$). Compared to the original GNN model that caches intermediate data from all P tasks (Figure 8(a)), the task-decoupled approach only requires reserving space for one P task, reducing the memory requirements. For complex GAT models, since the Scatter P task is executed before the edge T task, we must cache the edge embeddings generated by the Scatter P task, which consumes a significant memory resource. To address this challenge, we swap the execution order of the Scatter P task and the edge T task following the solution proposed by GATv2 [5], ensuring that all P tasks are executed consecutively so that release their intermediate data.

The flow of the task-decoupled approach is as follows. For the given L-layer GNN model, NeutronTask first separates all T tasks from P tasks and executes the task partition based on the separated L-layer T tasks and L-layer P tasks. Based on this, we load the subgraphs to execute the L-layer vertex-based T tasks and transfer the obtained vertex embeddings to the GPUs of P tasks. Subsequently, we execute L-layer P tasks, obtaining aggregated vertex embeddings and calculating the corresponding loss. Backward propagation involves executing the previous process in reverse, using the obtained vertex gradients instead of vertex embeddings.

Furthermore, we analyze the communication complexity of data parallelism, task parallelism, and task-decoupled approach. Let L be the number of layers, M be the number of GPUs, $|V|$ be the number of vertices, and $|d|$ be the average embedding dimension. For data parallelism, which only communicates neighbor vertices, the communication complexity is $O((\alpha-1)|V||L||d|)$, where $\alpha \geq 1$ represents the replication factor. For task parallelism, which transfers all vertex embeddings between the T and P tasks, the communication complexity is $O((2L-1)|V||d|)$. For task-decoupled, the communication complexity is $O((M-1))|V||d|)$. Since α is proportional to the average degree, datasets with a higher average degree exhibit greater communication volume in data parallelism. When $N_{GPU} < N_{task}$, the task-decoupled approach can effectively address the frequent communication issues inherent in the alternating execution mode, as shown in Figure 9.

Recomputation Technique. Based on task-decoupled GNN training, T tasks are grouped together for execution, and this part can be seen as a traditional DNN operation. Therefore, we can use

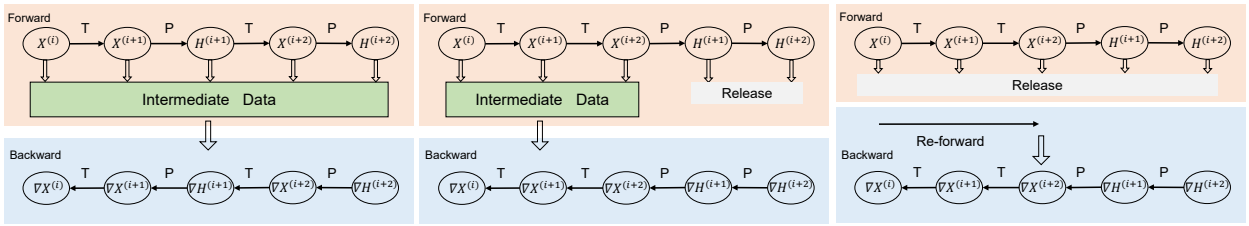

Figure 8: The data flow of different training methods. Ellipses represent tensors generated by each operation. The tensor pointing to the green area represents intermediate data that needs to be cached in GPU memory.

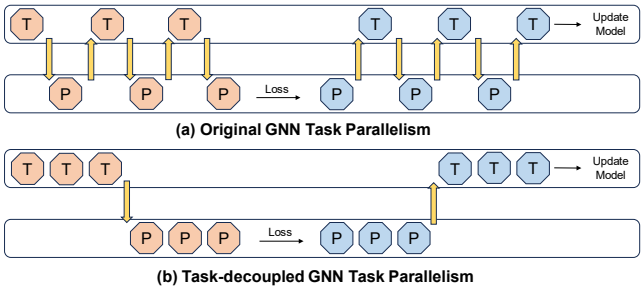

Figure 9: An illustrative example for comparing the communication frequency of original GNN task parallelism and task-decoupled GNN task parallelism (3-layer GNN).

recomputation techniques [12] to reduce the intermediate data generated by T tasks. As is illustrated in Figure 8(c), the recomputation technique involves re-executing the T tasks during backward propagation instead of caching their intermediate data, reducing the runtime memory consumption in decoupled GNN training.

NeutronTask implements the recomputation technique into task-decoupled GNN task parallelism to reduce memory consumption. In forward propagation, after each GPU completes the T task for a subgraph, it immediately releases all intermediate data to reserve memory space for the next subgraph. In backward propagation, each subgraph performs recomputation and gradient propagation in parallel (recomputing the T task starting from the first GPU and propagating gradients starting from the last GPU). Note that the recomputation technique maintains the accuracy of the original approach because the recomputed intermediate data are identical to that generated during forward propagation.

The Effectiveness of Task-Decoupled Approach. For data parallelism, the memory requirement for intermediate data is $ID_{dp} = 2 \cdot |V|L|d|$, where $|V|$ is the number of vertices, L is the model layers, and $|d|$ is the average dimension of hidden layers. For task-decoupled approach, intermediate data is released after performing tasks and the memory requirement is $ID_{tp} = |d| \sum_{i=m}^{n} |V_i|$, where m and n represent the subgraphs being processed. Since $\sum_{i=m}^{n} |V_i| < |V|$, we have $ID_{dp} < ID_{tp}$. Therefore, task-decoupled approach reduces memory requirement for intermediate data.

5.2 Task Scheduling Model

NeutronTask integrates task parallelism and task-decoupled GNN training framework, minimizing runtime memory consumption during GNN training. In this section, we provide a task scheduling model that optimizes GPU resource utilization by adjusting the number of GPUs allocated to each task based on the workload. Initially, we analyze the factors that affect the execution time of T and P tasks. Firstly, T tasks run slower on graphs with larger input feature dimensions, while P tasks run slower on graphs with higher average degrees. Secondly, T tasks are compute-intensive, with performance primarily related to computational resources, whereas P tasks are memory-intensive, primarily associated with memory access speed [53].

Based on the above analysis, we design a task scheduling model. Firstly, we estimate the computation time of T and P tasks in a given GNN workload using the following formulas:

$$T_t = \frac{\sum_{l=1}^{L} 2 \cdot |V| \cdot d_v^{(l)} \cdot d_v^{(l+1)} + 2 \cdot |E| \cdot d_e \cdot d_e}{\text{FLOPS}} \tag{5}$$

$$T_p = \sum_{l=1}^{L} \left(\gamma \cdot \frac{2 \cdot |V| \cdot \bar{d} \cdot d_v^{(l)}}{\text{FLOPS}} + (1-\gamma) \cdot \frac{|V| \cdot \bar{d} \cdot (1 + 2 \cdot d_v^{(l)}) + |V|}{\text{Bandwidth}} \right) \tag{6}$$

where L is the number of GNN layers, *e.g.*, L vertex-based T task, L P tasks, and an edge-based T task in complex models. $|V|$ and $|E|$ are the number of vertices and edges in the graph, respectively. $d_v^{(l)}$ is the embedding dimensions of the vertices and edges at layer l, and d_e represents the last layer of T tasks ($d_e = d_v^{(L)}$). $\bar{d}$ is the average degree of vertices in the graph. FLOPS denotes the computational capacity of the GPU in terms of floating-point operations per second. Bandwidth is the memory bandwidth. γ represents the extent to which computation and communication overlap, typically determined empirically based on hardware characteristics.

Based on these measurements, we calculate the number of GPUs allocated to P tasks (N_p) and T tasks (N_t) as follows:

$$N_p = N_g \cdot \frac{T_p}{T_p + T_t}, \tag{7}$$

$$N_t = N_g - N_p, \tag{8}$$

where N_g is the total number of available GPUs. By task scheduling model, NeutronTask ensures optimal performance and efficient utilization of available hardware. Additionally, the task scheduling model is a pre-processing phase. The complexity of task scheduling is constant and its overhead is relatively small, accounting for about 0.01% of the total time for running 100 epochs.

5.3 Overall Execution Flow in NeutronTask

Algorithm 2 outlines a single epoch's execution in NeutronTask. To begin with, GNN tasks are allocated by the task scheduling model. The $\{T_k | 0 < k < q\}$ and $\{P_k | q - 1 < k < N\}$ represent the number of T and P tasks in each GPU, N represents the number of GPUs, and q represents the boundary point for handling two types of GPU,

Algorithm 2 Workflow of NeutronTask for a single epoch.

Input: $G = (V, E)$, input feature $X^{(0)}$, Epoch e, the number of GPU N, the number of subgraph S
Output: Updated Parameter of GNN model W

1: $\{T_k|, 0 < k < q\}, \{P_k|, q < k < N\} = Task\_Partition(N, G)$;
2: ▷ P_k represents the number of P tasks in each GPU
3: $\{SG[i][j]|0 \le i, j < S\} = Graph\_Partition(G, S)$;
4: SyncALLGPU();
5: **for** each $s \in SG[i][j]$ **do in pipeline**
6: Transfer feature to the first "T" GPU, *i.e.,* $H_s^{(0)}$;
7: **for** $GPU\ k = 0$ to $q - 1$ **do**
8: $H_s^{(k)} = g_\theta(X_s, W_k, T_k)$ (or $\gamma = e_\theta(X_s, W_e)$);
9: Transfer $H_s^{(k)}$ to next "T" GPU;
10: **end for**
11: Transfer H from "T" GPU to first "P" GPU;
12: **for** $GPU\ k = q$ to $N - 1$ **do**
13: $H_s^{(k)} = f(\mathrm{H}, \hat{A}, P_k)$; // vertex dependency management
14: Transfer $H_s^{(k)}$ to next "P" GPU;
15: **end for**
16: loss = $downstream\_task(H_s^{(k)})$;
17: $\nabla H = loss.backward()$;
18: $Re\_forward()$; // from GPU 0 to $q - 1$
19: $P\_backward()$; // from GPU $N - 1$ to q
20: $T\_backward()$ and $Update(W)$;
21: **end for**

where GPUs with $GPU_{id} < q$ handle T tasks, and the remaining GPUs handle P tasks (line 1). Then, we employ intra-GPU graph partitioning to partition the input graph into multiple subgraphs (SG), where the organization of each SG resembles the chunk-based graph structure shown in Figure 6 (line 3).

Before the start of each epoch, all GPUs are synchronized (line 4). During the training process, SGs are trained sequentially within a GPU and scheduled with pipeline parallelism across GPUs. The feature $H_s^{(0)}$ is transferred from the host to the GPU executing the first T task (line 6). Then, the embeddings of each SG are transmitted across GPUs in the predetermined order, performing the corresponding tasks (lines 7-15). In backward propagation, recomputation (line 18) and gradient propagation (line 19) can be executed in parallel, ultimately updating the model parameters (line 20).

6 EXPERIMENTAL EVALUATION

6.1 Experimental Setup

Environments. The multi-GPU experiments are conducted on a GPU server equipped with 2 Intel(R) Xeon(R) Silver 4316 CPUs, 377GB DRAM, and 4 NVIDIA A5000 (24GB) GPUs. Each CPU is connected to two GPUs via the PCIe link, and the multi-GPU devices are connected with PCIe 4.0x 16. The server runs Ubuntu 20.04 OS with GCC-9.4.0, CUDA 11.3, PyTorch 1.13.0, and NCCL backend.

Datasets and GNN Algorithms. Table 3 presents the major parameters of real-world graphs used in our experiments. For graphs without ground-truth properties (it-2004 and friendster), we use randomly generated features, labels, training (25%), test (25%), and validation (50%) set division. We use two popular GNN models (GCN [29] and GAT [56]). The hidden layer dimensions for reddit and ogbn-products are set to 256, while for cora, it-2004, ogbn-papers100M, and friendster, they are set to 128. In our evaluation,

Table 3: Dataset description. |V|, |E|, #F, #L, and #hidden represent the number of vertices, edges, feature dimensions, and labels, respectively. |TR| represents the ratio of train vertices.

Dataset	|V|	|E|	#F	#L	|TR|
cora [45]	2.70K	5.43K	1433	7	59.3%
reddit [23]	232.96K	114.62M	602	41	90.6%
ogbn-products [26]	2.45M	61.86M	100	47	8.03%
it-2004 [4]	41M	1.2B	256	64	25%
ogbn-papers100M [26]	111.06M	1.62B	128	172	1.1%
friendster [31]	65.6M	2.5B	256	64	25%

the partition number is set to 4. Since it-2004, ogbn-papers100M, and friendster are large, their partitions are additionally split to 32.

System for Comparison. We compare NeutronTask with three popular GNN systems: DGL [62], NeutronStar [64], and Sancus [43], all of which employ data parallelism. DGL employs mini-batch training to reduce memory usage for large-scale graphs, where the training vertices are divided into multiple batches, and then each batch samples a subset of neighbors to load onto the GPU for training. In our evaluation, the batch size is set to 1024 and the fan-out for each layer is set to 10. NeutronStar adapts to large-scale graph training by dividing the entire graph into subgraphs and loading them sequentially into the GPU. Sancus reduces communication by using historical embeddings and caches these embeddings locally.

6.2 Overall Comparison

We compare NeutronTask with DGL [62], Sancus [43], and NeutronStar [64] on a node with 4 GPUs to show the processing scale with limited GPU resources. The results are reported in Table 4.

Compared to DGL, NeutronTask achieves an average speedup of 2.87×. The sampling method of DGL faces the neighbor explosion problem [27], where the computational and memory requirements of mini-batch GNN training grow exponentially with the number of model layers. Since DGL needs to store intermediate data, it encounters OOM errors when handling deep GNN models. In contrast, by utilizing the task-decoupled approach and recomputation techniques, NeutronTask can immediately release intermediate data after completing each layer of GNN tasks. Additionally, due to the time-consuming in the sampling process, DGL's training efficiency is lower than NeutronTask. For ogbn-papers100M, DGL shows better performance because it trains only on the training set, which accounts for just 1.1% of the total vertices. In contrast, NeutronTask performs full-graph GNN training, *i.e.,* all vertices participate in the training process, resulting in higher computational overhead.

Compared to Sancus and NeutronStar, NeutronTask not only supports large-scale graph training but also demonstrates superior performance. Sancus caches historical embeddings locally, significantly increasing memory requirements. Despite NeutronStar reducing the training data through subgraph partitioning, it still requires intermediate data to be stored entirely in GPUs. NeutronTask reduces the memory consumption by task parallelism and task-decoupled approach, enhances system performance by efficient pipeline parallelism. Firstly, NeutronTask reduces neighbor replication by avoiding inter-GPU graph partition and reduces intermediate data by decoupling T tasks from P tasks. As a result, NeutronTask can train on all datasets, while Sancus and NeutronStar are limited to small-scale graphs. Secondly, each GPU transmits its computation results

Table 4: Comparison of the per-epoch time (unit: s) with DGL, Sancus, and NeutronStar. (OOM represents out-of-memory)

Layers	Dataset	GCN				GAT			
		DGL	Sancus	NeutronStar	NeutronTask	DGL	Sancus	NeutronStar	NeutronTask
2	cora	0.025(3.13×)	0.017(2.13×)	0.013(1.66×)	0.008	0.021(2.1×)	0.023(2.3×)	0.028(2.8×)	0.010
	reddit	0.34(3.4×)	0.18(1.8×)	0.52(5.2×)	0.10	1.04(4.0×)	OOM	OOM	0.26
	ogbn-products	1.06(3.03×)	0.66(1.89×)	0.94(2.69×)	0.35	0.88(1.31×)	OOM	OOM	0.67
	it-2004	48.77(3.31×)	OOM	OOM	14.72	96.83(3.78×)	OOM	OOM	25.6
	ogbn-papers100M	2.76(0.13×)	OOM	OOM	25.88	10.71(0.2×)	OOM	OOM	54.84
	friendster	65.6(3.46×)	OOM	OOM	18.98	108.73(2.51×)	OOM	OOM	43.33
4	cora	0.044(2.32×)	0.03(1.58×)	0.05(2.63×)	0.019	0.0358(1.7×)	0.036(1.71×)	0.078(3.71×)	0.021
	reddit	0.625(3.29×)	0.36(1.89×)	0.92(4.84×)	0.19	1.96(5.45×)	OOM	OOM	0.36
	ogbn-products	1.378(2.46×)	1.82(3.25×)	1.75(3.13×)	0.56	3.86(4.71×)	OOM	OOM	0.82
	it-2004	64.4(3.45×)	OOM	OOM	18.69	OOM	OOM	OOM	47.43
	ogbn-papers100M	17.86(0.36×)	OOM	OOM	57.72	61.65(0.6×)	OOM	OOM	102.39
	friendster	OOM	OOM	OOM	35.31	OOM	OOM	OOM	75.95
8	cora	0.063(1.91×)	0.042(1.27×)	0.05(1.52×)	0.033	0.058(1.81×)	0.057(1.78×)	0.099(3.09×)	0.032
	reddit	1.546(4.83×)	0.71(2.22×)	1.75(5.47×)	0.32	OOM	OOM	OOM	0.41
	ogbn-products	OOM	OOM	6.23(5.32×)	1.17	OOM	OOM	OOM	1.58
	it-2004	96.45(2.58×)	OOM	OOM	37.45	OOM	OOM	OOM	77.85
	ogbn-papers100M	OOM	OOM	OOM	84.54	OOM	OOM	OOM	212.94
	friendster	OOM	OOM	OOM	77.71	OOM	OOM	OOM	152.96

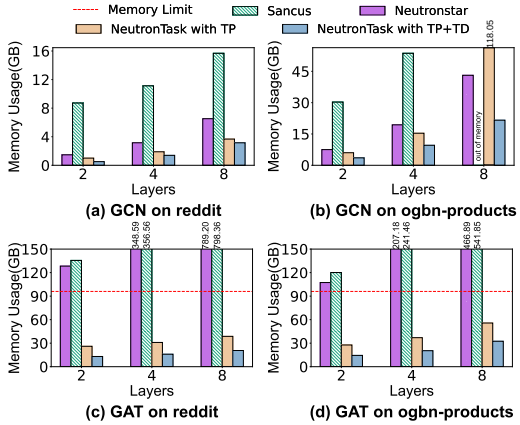

Figure 10: Memory reduction analysis, where each bar represents the peak memory consumption. "TP" indicates task parallelism, and "TD" indicates task-decoupled training.

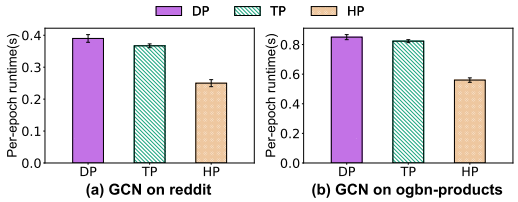

Figure 11: The performance comparison with error bars. The "DP" indicates data parallelism, "TP" indicates task parallelism, and "HP" indicates hybrid parallelism.

to the GPU handling the next task, allowing this communication to be hidden within the pipeline computations. On successfully runs, NeutronTask achieves a speedup from 1.27× to 5.47×.

Our observations indicate that the performance advantage of NeutronTask over other systems increases as the model layer grows. For the 2-layer model, NeutronTask achieves on average 2.37× speedup over the different systems. For the 4-layer model and 8-layer model, the speedups are 2.65× and 3.14×, respectively. This is because, as the number of layers increases, data parallelism need to manage more remote vertex dependencies (i.e., inter-GPU communication). In contrast, task parallelism reduces the communication overhead caused by vertex dependencies.

6.3 Memory Reduction Analysis

We analyze the memory reduction achieved by task parallelism (TP) and task-decoupled training (TD). We compare these approaches with NeutronStar [64] and Sancus [43] on two datasets. Figure 10 shows the total memory consumption across 4 GPUs.

NeutronStar consumes 19.9% – 43.7% of its memory to cache neighbor replication, while Sancus additionally caches historical embeddings by 32.7% – 43.3%. In contrast, NeutronTask reduces neighbor replication through TP. For reddit, TP reduces more neighbor replications than ogbn-products because it has a higher average degree, causing significant vertex dependencies across graph partitions. To cache the intermediate data, NeutronStar and Sancus consume 17.6% – 28.9% of the memory, whereas NeutronTask leverages TD to release this memory in advance. In addition, NeutronTask employs recomputation techniques to further reduce intermediate data of T tasks. For the GAT model, the memory requirements of both NeutronStar and Sancus exceed the total memory of four GPUs (96GB), and we compute their theoretical memory requirements. NeutronTask avoids storing a large number of edge embeddings by leveraging vertex weights for storage, which significantly reduces memory usage by 81.5% – 97.4%. In summary, compared to these systems, NeutronTask reduces total memory usage by 49% – 67%.

6.4 Efficiency of the Hybrid Parallelism

NeutronTask employs hybrid parallelism (HP) to address the scenario where the number of GPUs exceeds the number of tasks. We compare HP with data parallelism (DP) and task parallelism (TP) to analyze performance. We conduct the experiments on an Alibaba Cloud ECS server equipped with 128 vCPU cores, 512 GB of DRAM, and 8 A10 GPUs (each with 24 GB). The rest of the software setup is described in Section 6.1. We use a 2-layer GCN model, which

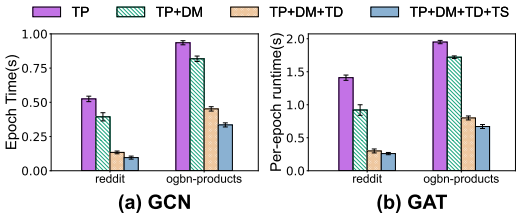

Figure 12: Performance gain analysis with error bars. "TP" indicates the naive task parallelism, "DM" indicates the vertex dependency management, "TD" indicates the task-decoupled GNN training, and "TS" indices the task scheduling model.

includes two P tasks and two T tasks. In this setup, DP uses NeutronStar as the baseline. TP only utilizes 4 GPUs. For HP, we evenly divide the GPUs into 4 groups, with each group handling one task. Both TP and HP do not include the task-decoupled approach. Figure 11 shows the experimental results of per-epoch time. Compared to DP, hybrid parallelism achieves a 1.52× - 1.56× speedup. This is because DP requires frequent communication with remote neighbors. However, HP reduces the communication overhead (achieved by reducing neighbor replications) and overlaps inter-GPU communication with computation between tasks. Compared to TP, HP achieves a 1.46× - 1.47× speedup. This is because TP uses only 4 GPUs for GNN training, leaving the other 4 underutilized. In contrast, HP maximizes GPU resource utilization by grouping GPUs.

6.5 Performance Gain Analysis

We analyze the performance gain of NeutronTask with vertex dependency management (DM), task-decoupled GNN training (TD), and task scheduling model (TS). We take naive task parallelism (TP) as the baseline and gradually integrate the three optimization approaches. Figure 12 shows the result. Compared to TP, TP+DM achieves speedups ranging from 1.6× - 1.8×. As illustrated in Figure 5, DM reduces GPU bubble time in task parallelism by overlapping the execution of subgraph tasks across GPUs. Compared to TP+DM, TP+DM+TD achieves speedups ranging from 1.8× - 2.9×, which is due to the inherent advantages of decoupled training. In the general GNN model, the P tasks perform computations using the vertex embeddings from each hidden layer. In contrast, TD first executes all T tasks, which may reduce the dimensions of vertex embeddings. The TD achieves greater performance gains for reddit than ogbn-products. This is because after T tasks, the vertex embedding dimensions in the reddit dataset sharply decrease, directly reducing the execution time of P tasks. For the GAT model, the performance gain introduced by TD is greater than that for the GCN model. This is because TD decouples the computation of edge weights for P and T tasks, further reducing the communication frequency across GPUs. Finally, compared to TP+DM+TD, TP+DM+TD+TS achieved speedups ranging from 1.35× - 1.39× by adjusting the number of GPUs executing different tasks, enhancing resource utilization.

6.6 Accuracy Comparison

NeutronTask employs task-decoupled GNN training that separates all T tasks from P tasks, executing L layers of T tasks first, followed by L layers of P tasks, which impact model accuracy. We compare the model accuracy of NeutronTask with DGL [62] and Sancus [43] by running GCN on reddit and ogbn-products. Figure 13 reports the epoch-to-accuracy results. After 100 epochs, the test accuracy reaches a stable state. NeutronTask achieves almost

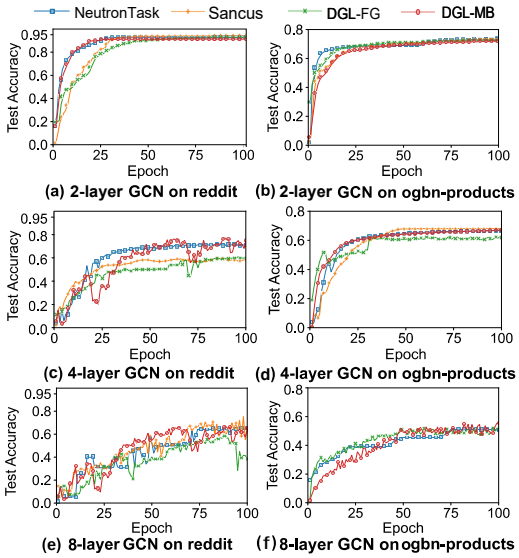

Figure 13: Epoch-to-accuracy. MB represents the mini-batch training, and FG represents the full-graph training.

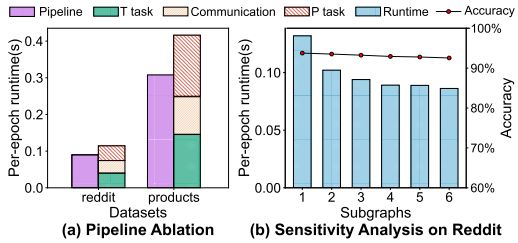

Figure 14: Pipeline performance and sensitivity analysis.

the same accuracy as other systems, demonstrating the effectiveness of task-decoupled GNN training in ensuring model accuracy. Regarding the convergence speed, NeutronTask achieves the highest accuracy in fewer epochs. Additionally, due to the per-epoch time of NeutronTask being significantly faster than other baselines, demonstrating better time-to-accuracy performance. Sancus has the slowest convergence speed due to the use of history embedding. For deeper layers, all methods suffer from decreased accuracy. This is because the increased number of P and T tasks leads to issues such as over-smoothing [7, 10, 16, 17, 40, 41, 69, 78] and over-fitting [32, 44, 70, 82]. Graphs with higher average degrees are more susceptible to over-smoothing. Therefore, reddit suffers from a more significant accuracy drop compared to ogbn-products.

6.7 Efficiency of Pipelining

We conduct pipeline ablation experiments to demonstrate the effectiveness of the pipeline and analyze the impact of the number of subgraphs on system performance and model accuracy.

Ablation Study of the Pipeline. To evaluate the efficiency of pipelining shown in Figure 5(c), we compare it with the serial execution of 4 subgraphs. Figure 14(a) shows the result, the time elapsed on both T and P tasks is roughly the same, which exceeds the time elapsed on communication. By overlapping the communication and computation through pipelining, the total runtime can be significantly reduced (ranging from 1.2× to 1.5×).

Sensitivity Study of the Pipeline. In intra-GPU graph partition, the number of subgraphs is a configurable parameter that

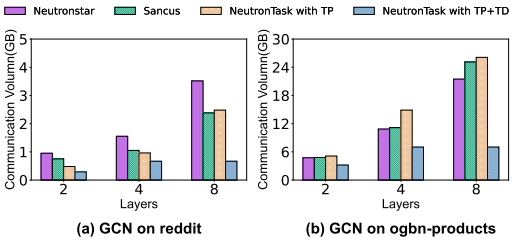

Figure 15: The average communication volume. "TP" represents task parallelism, and "TD" represents task-decoupled approach.

controls the memory consumption of training data and pipeline parallelism. To evaluate the impact of this parameter on training performance and accuracy, we run a 2-layer GCN on reddit, increasing the number of subgraphs from 1 to 6. As shown in Figure 14(b), as the number of subgraphs increases, the performance gradually improves, while accuracy decreases by less than 1%.

6.8 Communication Analysis

We evaluate the communication overhead of NeutronTask by integrating task parallelism (TP) and task-decoupled (TD). Figure 15 presents the experimental results compared to two full-graph data parallelism systems (NeutronStar and Sancus). For reddit, NeutronTask with TP reduces the communication overhead by an average of 36%, while for ogbn-products, NeutronTask with TP increases the communication overhead by an average of 17%. This is because, when data parallelism runs on datasets with a higher average degree (reddit), there are more cross-GPU edges, resulting in a higher communication volume. Compared to other methods, NeutronTask with TP+TD reduces communication column by an average of 54.2%. This is because TD involves fewer communication frequency.

6.9 Scalability Analysis

Scalability with Varying GPUs. We evaluate the scalability of NeutronTask by varying the number of GPUs. Figure 16 reports the experimental results of 2-layer GCN and GAT using DGL and Sancus as baselines. We observe that the performance of NeutronTask, DGL, and Sancus improves with the increase in the number of GPUs. NeutronTask leverages an efficient pipeline to achieve high scalability by overlapping computation and communication. Sancus has poor scalability because the increase in the number of GPUs leads to more graph partitions, resulting in more vertex dependencies and inter-GPU communication. For GAT, Sancus encounters an OOM error. DGL achieves high scalability because the total fixed number of batches and the increasing number of GPUs result in the number of batches processed by each GPU decreasing linearly.

Scalability with Varying Dataset Characteristics. We compare NeutronTask with DGL, NeutronStar, and Sancus by varying dataset characteristics. Specifically, we utilize the RMAT [28] to generate datasets and fix the number of vertices at 20M while varying the number of edges (#E, 80M, 160M, 320M), the feature dimensions (#F, 256, 512, 1024), the labels (#L, 16, 32, 64), and the ratio of train vertices ($|TR|$, 10%, 50%, 80%). The results are shown in Figure 17. With varying #E, #F, #L. $|TR|$, NeutronTask achieves speedup of 5.60×, 3.68×, and 4.52× compared to DGL, Sancus, and NeutronStar, respectively. The computational overhead of mini-batch training in DGL is proportional to $|TR|$, while the computational overhead of full-graph training is independent of $|TR|$.

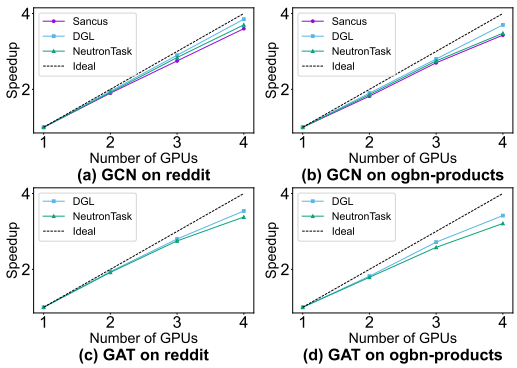

Figure 16: Scalability analysis when varying GPU number from 1 to 4 by running 2-layer GNN models.

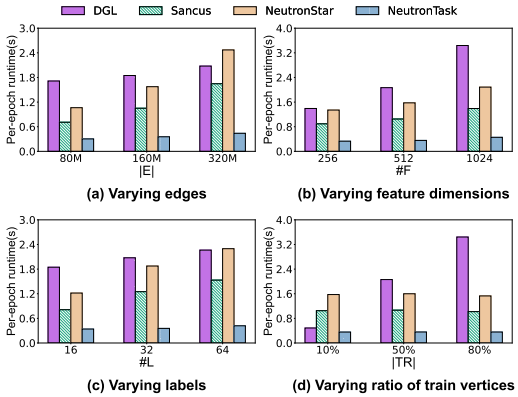

Figure 17: Scalability analysis when varying dataset characteristics when fixing the number of vertices at 20M.

6.10 GPU Utilization

We evaluate the GPU Utilization by running 2-layer GCN on reddit. Figure 18 reports the experimental results in a 0.7-second time window. GPU utilization is recorded every 1 millisecond. NeutronTask exhibits higher GPU utilization (97.24% on average) compared to DGL (94.65% on average), Sancus (97.11% on average), and NeutronStar (94.89% on average), with consistently higher peak GPU utilization for most of the time. This is because NeutronTask designs a flexible task scheduling model to adjust the number of GPUs allocated for T and P tasks based on their execution times. NeutronTask experiences some fluctuation due to the bubble time in the pipeline. DGL has the worst GPU utilization due to its sampling process, which involves many random memory accesses.

6.11 Comparison with NeutronTP

In this section, we compare NeutronTask with NeutronTP, which is based on tensor parallelism that evenly divides vertex features to achieve load balance. Moreover, we combine NeutronTask with tensor parallelism to demonstrate the performance of using both techniques, where GPUs are grouped to perform tensor parallelism within each group and task parallelism across groups. Figure 19 reports the experimental results with NeutronStar (data parallelism) as the baseline. Compared to NeutronStar, all methods improve performance. When training small-scale graphs, NeutronTP achieves an average speedup of 4.11× than NeutronTask. However, for large-scale graphs, the subgraph loading of NeutronTP reduces GPU utilization, leading to performance degradation, and even memory exhaustion errors, while NeutronTask achieves 4.21× speedup

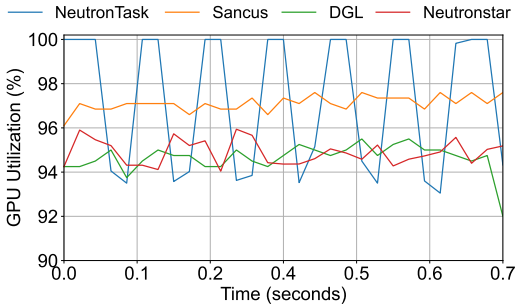

Figure 18: GPU utilization comparison. The average GPU utilizations are 97.24%, 97.11%, 94.65%, and 94.89% for NeutronTask, Sancus, DGL, and NeutronStar respectively.

on it-2004. After combining tensor parallelism, NeutronTask not only supports large-scale graph training but also further enhances performance. In summary, tensor parallelism and task parallelism are orthogonal techniques. Combining them can achieve better performance than using a single one.

7 LIMITATION AND FUTURE WORK

Currently, NeutronTask is primarily designed for training large-scale graphs in environments with limited GPU memory resources. When resources are adequate or the graph scale is relatively small, NeutronTask may need to be combined with other parallel methods to further enhance training performance.

Recently, various GNN parallel training methods, such as GNN tensor parallelism [2] and GNN model parallelism [59], have been proposed to balance workloads among workers and enhance inter-layer pipeline performance. However, evaluating the appropriate use cases for these methods and effectively combining them remains an open research problem. In future work, we aim to integrate existing parallelization techniques to enable automatic parallelism for GNNs. This framework would automatically select the most suitable execution strategy (or combine multiple parallelization methods) to adapt to varying requirements based on specific environments and data inputs.

8 RELATED WORK

Mini-batch GNN Systems. Some sampling-based GNN training systems have been proposed to solve the problems of limited GPU memory [1, 19, 33, 34, 46, 47, 51, 58, 71, 72, 76, 79, 80, 84]. GNNLab [72] efficiently utilizes GPU memory through a pre-sampling-based caching strategy. WholeGraph [71] eliminates CPU-GPU communication by scattering data across multiple GPUs and accelerates data access using GPUDirect P2P memory access. DUCATI [76] reduces host-GPU data transfers by using GPU caching for graph topology and features. MariusGNN [58] utilizes the entire storage hierarchy (including disk) for out-of-core GNN training. P3 [19] utilizes feature slices to complete the first P tasks to reduce communication overhead. ByteGNN [79] and PaGraph [34] employ streaming partitioning to generate the optimal graph partition. XGNN [51] designs a Global GNN Memory Store to fully utilize system memory and high-speed inter-GPU interconnects. DAHA [33] explores the optimal execution plan under CPU-GPU heterogeneous environments by a data and hardware aware cost model. OUTRE [47] designs partition-based batch construction and historical embedding cache

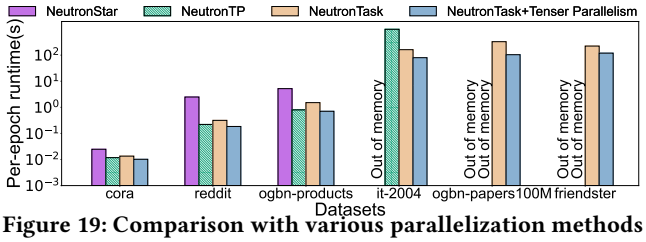

Figure 19: Comparison with various parallelization methods

to reduce the neighborhood redundancy and temporal redundancy that exists in out-of-core sample-based GNN training.

Full-graph GNN Training. A set of GNN systems [8, 27, 38, 43, 54, 59, 60, 63–65, 77] adopt full-graph GNN training to guarantee high accuracy. CAGNET [54] proposes 1.5D, 2D, and 3D sparse-dense matrix multiplication to optimize data distribution between GPUs. Sancus [43] explores using staleness embedding in GNN training to reduce communication frequency while maintaining accuracy instead of transmitting them each epoch. MGG [65] implements a fine-grained pipeline for communication and computation between remote and local vertices, which aims to overlap communication and computation times through GPU warp allocation. ROC [27] uses a cost model to represent host-GPU data transfer overhead and employs dynamic programming to find the optimal communication plan. G3 [60] propose GNN hybrid parallelism to scale out GNN training with carefully scheduled peer-to-peer intermediate data sharing. Lotan [77] bridges the siloed worlds of graph analytics systems and DL systems. PipeGCN [59] hides the communication overhead by pipelining inter-partition communication with intra-partition computation on distributed GCN training.

GNN Tensor Parallelism. Recently, NeutronTP [2] proposes tensor parallelism, ensuring that different workers process nearly identical workloads by partitioning vertex tensors instead of partitioning graphs (as vertex tensors have equal sizes and are easier to partition evenly). To address frequent communication, NeutronTP proposes a general decoupled training technique. In contrast, we employ decoupled training based on task parallelism, releasing intermediate data in advance to reduce memory requirements.

9 CONCLUSION

We present NeutronTask, a scalable and efficient system for full-graph GNN training on limited GPU memory. Firstly, NeutronTask provides task parallelism, which reduces neighbor replication and reorganizes intermediate data placement in multi-GPU GNN training by inter-GPU task partition and intra-GPU graph partition. Secondly, NeutronTask integrates a task-decoupled GNN training framework, which reduces the intermediate data in GNN training through task-decoupled GNN training and recomputation techniques. Our experiments demonstrate that NeutronTask can efficiently train on billion-scale graphs using just 4×A5000 GPU (each with 24GB of memory) by significantly reducing the memory consumption of neighbor replication and intermediate data.

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