GOSH: Embedding Big Graphs on Small Hardware

Taha Atahan Akyildiz* aakyildiz@sabanciuniv.edu Sabanci University Amro Alabsi Aljundi* amroa@sabanciuniv.edu Sabanci University Kamer Kaya Sabanci University kaya@sabanciuniv.edu

ABSTRACT

In graph embedding, the connectivity information of a graph is used to represent each vertex as a point in a *d*-dimensional space. Unlike the original, irregular structural information, such a representation can be used for a multitude of machine learning tasks. Although the process is extremely useful in practice, it is indeed expensive and unfortunately, the graphs are becoming larger and harder to embed. Attempts at scaling up the process to larger graphs have been successful but often at a steep price in hardware requirements. We present GOSH, an approach for embedding graphs of arbitrary sizes on a single GPU with minimum constraints. GOSH utilizes a novel graph coarsening approach to compress the graph and minimize the work required for embedding, delivering high-quality embeddings at a fraction of the time compared to the state-of-the-art. In addition to this, it incorporates a decomposition schema that enables any arbitrarily large graph to be embedded using a single GPU with minimum constraints on the memory size. With these techniques, GOSH is able to embed a graph with over 65 million vertices and 1.8 billion edges in less than an hour on a single GPU and obtains a 93% AUCROC for link-prediction which can be increased to 95% by running the tool for 80 minutes.

CCS CONCEPTS

• Parallel computing methodologies → Parallel algorithms; Shared memory algorithms; • Mathematics of computing → Discrete mathematics; Graph theory; Graph algorithms.

KEYWORDS

Graph embedding, GPU, parallel graph algorithms, graph coarsening, link prediction

ACM Reference Format:

Taha Atahan Akyildiz, Amro Alabsi Aljundi, and Kamer Kaya. 2020. GOSH: Embedding Big Graphs on Small Hardware. In 49th International Conference on Parallel Processing - ICPP (ICPP '20), August 17–20, 2020, Edmonton, AB, Canada. ACM, New York, NY, USA, 11 pages. https://doi.org/10.1145/ 3404397.3404456

ICPP '20, August 17-20, 2020, Edmonton, AB, Canada

1 INTRODUCTION

Graphs are widely adopted to model the interactions within reallife data such as social networks, citation networks, web data, etc. Recently, using machine learning (ML) tasks such as link prediction, node classification, and anomaly detection on graphs became a popular area with various applications from different domains. The raw connectivity information of a graph, represented as its adjacency matrix, does not easily lend itself to be used in such ML tasks; regular *d*-dimensional representations are more appropriate for learning valid correlations between graph elements. Unfortunately, the connectivity information does not have such a structure. Recently, there has been a growing interest in the literature in the *graph embedding* problem which focuses on representing the vertices of a graph as *d*-dimensional vectors while embedding its structure into a *d*-dimensional space.

Various graph embedding techniques [6, 17, 21, 22] have been proposed in the literature. However, these approaches do not usually scale to large, real-world graphs. For example, VERSE [22], deepwalk [17], node2vec [6] and LINE [21] require hours of CPU training, even for small- and medium-scale graphs. Although these approaches can be parallelized, a multi-core CPU implementation of VERSE takes more than two hours on 16 CPU cores for a graph with 2 million vertices and 20 million edges. There are other attempts to increase graph embedding performance. HARP [3] and MILE [10] apply graph coarsening, a process in which a graph is compressed into smaller graphs, to make the process faster, but they do not have a parallel implementation. Accelerators such as GPUs can be used to deal with large-scale graphs. However, to the best of our knowledge, the only GPU-based tool in the literature is GRAPHVITE. Although GRAPHVITE is faster than the CPU counterparts, its use is limited by the device memory and it cannot embed large graphs with a single GPU.

In this paper, we present $GOSH^1$; an algorithm that performs parallel coarsening and many-core parallelism on GPU for fast embedding. The tool is designed to be fast and accurate and to handle large-scale graphs even on a single GPU. However, it can easily be extended to the multi-GPU setting. GOSH performs the embedding in a multilevel setting by using a novel, parallel coarsening algorithm which can shrink graphs while preserving their structural information and trying to avoid giant vertex sets during coarsening. With coarsening, the initial graph is iteratively shrunk into multiple levels. Then, starting from the smallest graph, unsupervised training is performed on the GPU. The embedding obtained from the current level is directly copied to the next one by using the coarsening information obtained from the above level. The process continues with the expanded embedding for the next level until the original graph is processed on the GPU and the final embedding is obtained. The contributions can be summarized as follows:

^{*}Both authors contributed equally to this research.

Permission to make digital or hard copies of all or part of this work for personal or classroom use is granted without fee provided that copies are not made or distributed for profit or commercial advantage and that copies bear this notice and the full citation on the first page. Copyrights for components of this work owned by others than the author(s) must be honored. Abstracting with credit is permitted. To copy otherwise, or republish, to post on servers or to redistribute to lists, requires prior specific permission and/or a fee. Request permissions from permissions@acm.org.

^{© 2020} Copyright held by the owner/author(s). Publication rights licensed to ACM. ACM ISBN 978-1-4503-8816-0/20/08...\$15.00 https://doi.org/10.1145/3404397.3404456

¹The code is publicly available at https://github.com/SabanciParallelComputing/GOSH

- To the best of our knowledge, the only GPU-based graph embedding tool, *GRAPHVITE*, cannot handle embedding large graphs on a single GPU when the total size of the embedding is larger than the total available memory of the GPU. On the contrary, *GOSH* applies a smart decomposition, update scheduling, and synchronization to perform the embedding even when the memory requirement exceeds the memory available on a single GPU.
- Thanks to multilevel coarsening and smart work distribution across levels, *GOSH*'s embedding is ultra-fast. For instance, on the graph com-lj, *GRAPHVITE*, a state-of-the-art GPU-based embedding tool, spends around 11 minutes to reach 98.33% AUCROC score. On the same graph, *GOSH* spends only 2.5 minutes and obtains 98.46% AUCROC score. Furthermore, based on the numbers given in [23], the embedding takes more than 20 hours on 4 Tesla P100 GPUs for a graph of 65 million vertices and 1.8 billion edges (the link prediction scores are not reported in [23] for this graph). On a single Titan X GPU, *GOSH* reaches 95% AUCROC score within 1.5 hours.
- The dimension, i.e., the number of features, used for the embedding process can vary with respect to the application. For different *d* values, the best possible GPU-implementation, which utilizes the device cores better, also differs. For different *d* values, *GosH* performs different parallelization strategies to further increase the performance of embedding especially for small *d* values.
- The multilevel setting for graph embedding has been previously applied by *MILE* [10] and *HARP* [3]. Since CPU-based embedding takes hours, the coarsening literature suggests that the time required for coarsening is negligible in comparison. In this work, we show that a parallel coarsening algorithm is necessary since *GOSH* is orders of magnitude faster than CPU-based approaches. To overcome this bottleneck, we propose an efficient and parallel coarsening algorithm which is empirically much faster than that of *MILE* and *HARP*.

The rest of the paper is organized as follows: In Section 2, the notation used in the paper is given. Section 3 describes *GosH* in detail including the coarsening algorithm and the techniques designed and implemented to handle large graphs. The experimental results are presented in Section 4 and the related work is summarized comparatively in Section 5. Section 6 concludes the paper.

2 NOTATION AND BACKGROUND

A graph G = (V, E) has V as the set of nodes/vertices and $E \subseteq (V \times V)$ as the set of edges among them. For undirected graphs, an edge is an unordered pair while in directed graphs, the order is significant. An embedding of a graph G = (V, E) is a $|V| \times d$ matrix **M**, where d is the dimension of the embedding. The vector $\mathbf{M}[i]$ corresponds to a vertex $i \in V$ and each value j in the vector $\mathbf{M}[i][j]$ captures a different feature of vertex i. The embedding of a graph can be used in many machine learning tasks such as link prediction [11], node classification [17] and anomaly detection [7].

There are many algorithms in the literature for embedding the nodes of a graph into a d-dimensional space. *GosH* implements the embedding method of *VERSE* [22]; a method which, in addition to

Taha Atahan Akyildiz, Amro Alabsi Aljundi, and Kamer Kaya

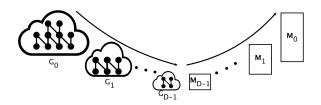


Figure 1: Multilevel embedding performed by *GOSH*: first, the coarsened set of graphs are generated. Then, the embedding matrices are trained until M₀ is obtained.

having fast run-time and low memory overhead, is highly generalizable as it can produce embeddings that reflect *any* vertex-to-vertex similarity measure Q. To elaborate, this approach defines two distributions for each vertex v: The first, sim_Q^v , is obtained from the similarity values between v and every other vertex in G computed based on Q. The second, $sim_{E^*}^v$ is derived from the embedding by using the cosine similarities of v's embedding vector and those of every other vertex in G. A soft-max normalization is applied to these values as a post-processing step so they sum up to 1. The problem then becomes the minimization of the Kullback-Leibler (KL) divergence between the two distributions for every vertex. In this paper, we choose Q to be the adjacency similarity measure described in [22].

Algorithm 1: UpdateEmbedding
Data: M[v], M[sample], b, lr
Result: M[v], M[sample]
1 score $\leftarrow b - \sigma(\mathbf{M}[v] \odot \mathbf{M}[sample]) \times lr$
² $M[v] \leftarrow M[v] + M[sample] \cdot score$
$3 M[sample] \leftarrow M[sample] + M[v] \cdot score$

The training procedure employs Noise Contrastive Estimation for convergence of the objective above as described in [22]. The process trains a logistic regression classifier to separate vertex samples drawn from the empirical distribution Q and vertex samples drawn from a noise distribution N, with the corresponding embedding vectors being the parameters of this classifier. More precisely, all the vertices are processed a total number of *e* times, i.e., *epochs*, where processing a vertex $v \in V$ consists of drawing a single positive sample *u* from sim_O^v and n_s negative samples $s_1, s_2, \ldots, s_{n_s}$ from *N*. In the meantime, logistic regression is used to minimize the negative log-likelihood of observing *u* and not observing $s_1, s_2, \ldots, s_{n_s}$ by updating the corresponding embedding vectors of v and all the other samples. A single update is shown in Algorithm 1, where M[v] is the embedding vector of v, M[sample] is the embedding vector of the sample, b is a binary number that is 1 if the sample is positive (drawn from Q) or negative (drawn from N), \odot is the dotproduct operation, σ is the sigmoid function and lr is the learning rate of the classifier.

The notation used in the paper is given in Table 1.

3 EMBEDDING ON SMALL HARDWARE

This section is organized as follows: First, a high-level explanation of GOSH is provided. Then, Section 3.1 describes the GPU GOSH: Embedding Big Graphs on Small Hardware

Table 1: Notation used in the paper.

Symbol	Definition
$G_0 = (V_0, E_0)$	The original graph to be embedded.
$G_i = (V_i, E_i)$	Represents a graph, which is coarsened <i>i</i> times.
$\Gamma^+(u)$	The set of outgoing neighbors of vertex <i>u</i> .
$\Gamma^{-}(u)$	The set of incoming neighbors of vertex <i>u</i> .
$\Gamma(u)$	Neighborhood of <i>u</i> , i.e., $\Gamma_{G_i}^+(u) \bigcup \Gamma_{G_i}^-(u)$.
d	# features per vertex, i.e., dimension of the embedding.
n _s	# negative samples per vertex.
σ	Sigmoid function.
sim _m	Similarity metric used in training.
е	Total number of epochs that will be performed
lr	Learning rate.
D	Total amount of coarsening levels.
G	The set of coarsened graphs created from a graph $G = G_0$.
p	Smoothing ratio for epoch distribution.
ei	# epochs for coarsening level <i>i</i> .
M_i	Embedding matrix obtained for G_i .
\mathcal{M}	The set of mappings used in coarsening.
тар _і	Mapping information from G_{i-1} to G_i .
V_i	The partitioning of vertex set V_i .
\mathcal{P}_i	The partitioning of embedding matrix M_i .
Ki	# parts in \mathcal{V}_i .
P_{GPU}	# embedding parts to be placed on the GPU.
S_{GPU}	# sample pools to be placed on the GPU.
В	# positive samples per vertex in a single sample pool.

implementation for the embedding process in detail. Following the embedding process, in Section 3.2, a new coarsening approach is introduced and the parallel implementation details are provided. Finally, Section 3.3 describes the partitioning schema which enables *GosH* to handle graphs that do not fit on the GPU memory.

Given a graph G_0 , GOSH, shown in Algorithm 2, computes the embedding matrix \mathbf{M}_0 . This is done in two stages;

- (1) creating a set *G* = {*G*₀, *G*₁,..., *G*_{*D*-1}} of graphs coarsened in an iterative manner (as in the left of Figure 1) where one or more than one nodes in *G*_{*i*-1} are represented by a super node in *G_i* (Line 1),
- (2) starting from G_{D-1} , training the embedding matrix \mathbf{M}_i for the graph G_i and projecting it to G_{i-1} to later train \mathbf{M}_{i-1} (as in the right of Figure 1) (Lines 3- 11).

The training process is repeated until \mathbf{M}_0 is obtained. To obtain \mathbf{M}_{i-1} from \mathbf{M}_i the mapping information of \mathbf{G}_{i-1} is used, where $M_i[u] = M_{i-1}[v]$ iff $u \in V_i$ is a super node of $v \in V_{i-1}$.

GOSH provides support for large-scale graphs for which the memory footprint of the training exceeds the device memory. Even for practical sizes, e.g., |V| = 128M and d = 128, the number of entries in the matrix is approximately 16G. With double precision, one needs to have 128GB memory on the device to store the entire matrix. For each G_i , *GOSH* initially checks if both G_i and M_i can fit in the GPU (Line 5). If so, it proceeds by copying G_i and the projection of M_i to the GPU and carrying out the embedding of G_i in a single step (Lines 6-7). Otherwise, it generates positive samples in CPU and carries out the embedding of G_i by copying the relative portions of the samples and M_i and training the graph in batches (Line 10).

Using multilevel coarsening arises an interesting problem; let e be the total number of epochs one performs on all levels. With a naive approach, one can distribute the epochs evenly to each level. However, when more epochs are reserved for G_i s in the lower levels, the process will be faster. To add, the corresponding embedding matrices will have a significant impact on the overall process as they are projected to further levels. On the other hand, when more epochs are reserved for the higher levels, i.e., larger G_i s, the embedding is expected to be more fine-tuned. So the question is how to distribute the epoch budget to the levels. Based on our preliminary experiments, GOSH employs a mixed strategy; a portion, p, of the epochs are distributed uniformly and the remaining $(e \times (1 - p))$ epochs are distributed geometrically. That is, training at level i uses $e_i = e/D + e'_i$ epochs where e'_i is half of e'_{i+1} . The value *p* is called the smoothing ratio and is left as a configurable parameter for the user to establish an interplay between the performance and accuracy.

Another parameter that has a significant impact on embedding quality is the learning rate. For multilevel embedding, a question that arises is *how to set the learning strategy for each level.* In *GOSH*, we use the same initial learning rate for each level, i.e., for the training of each \mathbf{M}_i and decrease it after each epoch. That is, the learning rate for epoch *j* at the *i*th level is equal to $lr \times \max\left(1 - \frac{j}{e_i}, 10^{-4}\right)$.

Algorithm 2: GOSH

8
Data: G_0 , n_s , lr , lr_d , p , e , threshold, P_{GPU} , S_{GPU} , B
Result: M
1 $\mathcal{G} \leftarrow \text{MultiEdgeCollapse}(G_0, threshold)$
² Randomly initialize M_{D-1}
3 for <i>i</i> from $D - 1$ to 1 do
$4 e_i \leftarrow \text{calculateEpochs}(e, p, i)$
5 if G_i and \mathbf{M}_i fits into GPU then
6 CopyToDevice (G_i, \mathbf{M}_i)
7 $M_i \leftarrow \text{TRAININGPU}(G_i, \mathbf{M}_i, n_s, lr, lr_d, e_i)$
8 else
9 $\mathbf{M}_i \leftarrow \text{LargeGraphGPU}(G_i, \mathbf{M}_i, n_s, lr, lr_d, e_i,$
10 P_{GPU}, S_{GPU}, B
11 $M_{i-1} \leftarrow \text{ExpandEmbedding}(M_i, map_{i-1})$
12 return M ₀

3.1 Graph embedding in GOSH

GOSH implements a GPU parallel, lock-free learning step for the embedding algorithm. As mentioned above, following *VERSE*, we use an SGD-based optimization process for training. As shown in [14], a lock-free implementation of SGD, which does not take the race conditions, i.e., simultaneous updates, into account, does not have a significant impact on the learning quality of the task on multi-core processors. However, our preliminary experiments show that on a GPU, where millions of threads are being executed in parallel, such race conditions significantly deteriorate the quality of the embedding. For *GOSH*, we follow a slightly more restricted implementation which is still not race-free.

To reduce the impact of race conditions, we synchronize the epochs and ensure that no two epochs are processed at the same time. For an epoch to train \mathbf{M}_i , *GOSH* traverses V_i in parallel by assigning a single vertex to a single GPU-warp. For a single (source) vertex, multiple positive and negative samples are processed one after another and updates are performed as in Algorithm 1. With this implementation and vertex-to-warp assignment, a vertex $v \in V_i$ cannot be a source vertex for two concurrent updates but it may be (positively or negatively) sampled by another vertex while the warp processing v is still active. Similarly, v can be sampled by two different source vertices at the same time. Hence, the reads/writes on $\mathbf{M}_i[v]$ are not completely race free. However, according to our experiments, synchronizing the epochs and samples for the same source vertex is enough to robustly perform the embedding process.

As shown in Algorithm 3, the positive and negative samples are generated in the GPU. For a source vertex $v \in V_i$, the positive sample $u \in V_i$ is chosen from $\Gamma_{G_i}(v)$. Negative samples, on the other hand, are drawn from a noise distribution as mentioned in Section 2 which we model as a uniform random distribution over V_i . After each sampling, the corresponding update is performed by using the procedure in Algorithm 1.

Al	gorithm 3: TrainInGPU
D	Data: G_i , \mathbf{M}_i , n_s , lr , e_i
R	Result: M _i
1 f	$\mathbf{or} \ j = 0 \ to \ e_i - 1 \ \mathbf{do}$
2	$lr' \leftarrow lr \times max\left(1 - \frac{j}{e_i}, 10^{-4}\right)$
	<pre>/* Each src below is assigned to a GPU warp */</pre>
3	for $\forall src \in V_i$ in parallel do
4	$u \leftarrow \text{GetPositiveSample}(G_i)$
5	UpdateEmbedding($M_i[src], M_i[u], 1, lr'$)
6	for $k = 1$ to n_s do
7	$u \leftarrow \text{GetNegativeSample}(G_i)$
8	UpdateEmbedding($M_i[src], M_i[u], 0, lr'$)

During the updates for a source vertex *src*, the threads in the corresponding warp perform $(1 + n_s) \times d$ accesses to $M_i[src]$. For large values of n_s and d, performing this many global memory accesses dramatically decreases the performance. To mitigate this, before processing *src*, *GosH* copies $M_i[src]$ from global to shared memory. Then for all positive and negative samples, the reads and writes for the source are performed on the shared memory. Finally, $M_i[src]$ is copied back to global memory. On the other hand, for the sampled *u* vertices, $M_i[u]$ is always kept in global memory since each entry is read and written only once. To perform coalesced accesses on $M_i[u]$, the reads and writes are performed in a roundrobin fashion. That is $M_i[u][j + (32 \times k)]$ is accessed by thread *j* at the *k*th access where 32 is the number of threads within a warp.

3.1.1 Embedding for small dimensions. Assuming a warp contains 32 threads, when $d \leq 16$ dimensions are used for embedding, a single source vertex does not keep all the threads in a warp busy. In this case, 32 - d warp threads remain idle which yields to the under-utilization of the device. To tackle this problem, we integrate a specialized implementation for small dimension embedding. We set the number of threads responsible for a source vertex as the

smallest multiple of 8 larger than or equal to *d*, i.e., 8 or 16. Hence, depending on *d*, we can assign 2 or 4 vertices to a single warp.

3.2 Graph coarsening

GOSH employs a fast algorithm to keep the structural information within the coarsed graphs while maximizing the coarsening *efficiency* and *effectiveness*. Coarsening efficiency at the *i*th level is measured by the rate of shrinking defined as $(|V_{i-1}| - |V_i|)/|V_{i-1}|$. On the other hand, the effectiveness is measured in terms of its embedding quality compared to other possible coarsenings of the same graph embedded with the same parameters. We adapt an agglomerative coarsening approach, MULTIEDGECOLLAPSE, which generates vertex clusters in a way similar to the one used in [3]. Given $G_i = (V_i, E_i)$, the vertices in V_i are processed one by one. If v is not marked, it is marked, and mapped to a cluster, i.e., a new vertex in V_{i+1} and its edges are processed. If an edge $(v, u) \in E_i$, where u is not marked, u is added to v's cluster. Then, all of the vertices in v's cluster are shrunk into a *super* vertex $v_{sup} \in G_{i+1}$.

MULTIEDGECOLLAPSE preserves both the first- and second-order proximites [21] in a graph. The former measures the pairwise connection between vertices, and the latter represents the similarity between vertices' neighborhoods. It achieves that by collapsing vertices that belong to the same neighborhood around a local, hub vertex. However, if this process is handled carelessly, two, giant hub vertices can be merged. We observed that this degrades the effectiveness and efficiency of the coarsening. The effectiveness degrades since the structural equivalence is not preserved in the lower levels of the coarsening, where most of the vertices are represented by a small set of super vertices. Furthermore having a small set of giant supers inhibits the graph from being coarsened further, resulting in an insufficient efficiency. To mitigate this, a new condition for matching is introduced to the algorithm, where $u \in V_i$ can not be put into the cluster of $v \in V_i$ if $|\Gamma_{G_i}(u)|$ and $|\Gamma_{G_i}(v)|$ are both larger than $\frac{|E_i|}{|V_i|}$. Consequently, assuming that the hub vertices will have a higher degree than the density of G_i , two of them can no longer be in the same cluster. Our preliminary experiments show that this simple rule has a significant effect on both the efficiency and the effectiveness of the coarsening.

As mentioned above, when a vertex is marked and added to a cluster, its edges are not processed further and it does not contribute to the coarsening. Performing the coarsening with an arbitrary ordering may degrade the efficiency since large vertices can be locked by the vertices with small neighborhoods. Hence, when an edge $(u, v) \in E_i$ is used for coarsening for a hub-vertex $v \in V_i$, to maximize efficiency, we prefer $u \in V_i$ to be inserted in to the cluster of origin v. To provide this, an ordering is procured by sorting the vertices with respect to their neighborhood size and this ordering is used during coarsening. This ensures processing vertices with a higher degree before the vertices with smaller neighborhoods and this results in a substantial increase in the coarsening efficiency.

The details of the coarsening phase are given in Algorithm 4. The algorithm takes an uncoarsened graph $G = G_0$ and returns the set of coarsened graphs G along with the mapping information to be used to project the embedding matrices \mathcal{M} . G and \mathcal{M} are initialized as $\{G_0\}$ and empty set, respectively. Starting from i = 0, the coarsening continues until a graph G_{i+1} with less than *threshold* vertices is generated. As mentioned above, first the vertices in G_i are sorted with respect to their neighborhood sizes. Then the coarsening is performed and a smaller G_{i+1} is generated. We also store the mapping information map_i used to shrink G_i to G_{i+1} . This will be used later to project the embedding matrix M_{i+1} obtained for G_{i+1} to initialize the matrix M_i for G_i . To add, *threshold* = 100 is used for all the experiments in the paper which is the default value for *GOSH*.

Algorithm 4: MultiEdgeCollapse
Data: $G_0 = (V_0, E_0)$, threshold
Result: \mathcal{G}, \mathcal{M}
$ 1 \ \mathcal{G} \leftarrow \{G_0\}, \mathcal{M} \leftarrow \emptyset, i \leftarrow 0 $
2 while $ V_i > threshold$ do
$order \leftarrow Sort(G_i)$
4 for $v \in V_i$ do $map_i[v] \leftarrow -1$
$\delta \leftarrow E_i / V_i $
$6 cluster \leftarrow 0$
7 for v in order do
s if $map_i[v] = -1$ then
9 $map_i[v] \leftarrow cluster$
10 $cluster \leftarrow cluster + 1$
11 foreach $(v, u) \in E_i$ do
12 if $ \Gamma_{G_i}(v) \leq \delta$ or $ \Gamma_{G_i}(u) \leq \delta$ then
$\begin{array}{c c c c c c c c c c c c c c c c c c c $
14 $\ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \$
15 $G_{i+1} \leftarrow \text{COARSEN}(G_i, map_i)$
16 $\mathcal{G} \leftarrow \mathcal{G} \cup \{G_{i+1}\}, \mathcal{M} \leftarrow \mathcal{M} \cup \{map_i\}, i \leftarrow i+1$

3.2.1 Complexity analysis: All the algorithms, coarsening and embedding, use the Compressed Sparse Row (CSR) graph data structure. In CSR, an array, *adj* holds the neighbors of every vertex in the graph consecutively. It is a list of all the neighbors of vertex 0, followed by all the neighbors of vertex 1, and so on. Another array, *xadj*, holds the starting indices of each vertex's neighbors in *adj*, with the last index being the number of edges in the graph. In other words, the neighbors of vertex *i* are stored in the array *adj* from *adj*[*xadj*[*i*]] until *adj*[*xadj*[*i* + 1]].

MULTIEDGECOLLAPSE has three stages; sorting (line 3), mapping (lines 7–14) and coarsening (line 15). A *counting sort* is implemented for the first stage with a time complexity of O(|V| + |E|). For mapping, the algorithm traverses all the edges in the graph. This has a time complexity of O(|V| + |E|). Finally, coarsening the graph requires sorting the vertices with respect to their mappings and going through all the vertices and their edges within the CSR, which also has a time complexity of O(|V| + |E|).

3.2.2 Parallelization: When the embedding is performed on the CPU, as the literature suggests, embedding dominates the total execution time. However, with fast embedding as in *GOSH*, this is not the case. Thus, we parallelize the coarsening on the CPU.

In a parallel coarsening with τ threads, one can simply traverse V_i in parallel and perform the mapping with no synchronization.

However, this creates race conditions and inconsistent coarsenings. To avoid race conditions, we use a lock per each entry of map_i . To update $map_i[v]$ and $map_i[u]$ as in lines 9 and 14, the thread first tries to lock $map_i[v]$ and $map_i[u]$, respectively. If the lock is obtained, the process continues. Otherwise, the thread skips the current candidate and continues with the next vertex. One caveat is the update on the counter *cluster*. Hence, instead of using a separate variable for super vertex ids, the parallel version uses the hub-vertex id for mapping. That is $map_i[v]$ is set to v unlike line 9 of the sequential algorithm. Note that with this implementation, map_i does not provide a mapping to actual vertex IDs in G_{i+1} . This can be fixed in O(|V|) time via sequential traversals of the $map_i[v] = v$ and reset the map_i values for all.

The parallel coarsened graph construction is not straightforward. After the mapping, the degrees of the (super) vertices in G_{i+1} are not yet known. To alleviate that, we allocate a private E_{i+1}^j region in the memory to each thread t_j , $1 \le j \le \tau$. These threads create the edge lists of the new vertices on these private regions which are then merged on a different location of size $|E_{i+1}|$. To do that first a sequential scan operation is performed to find the region in E_{i+1} for each thread. Then the private information is copied to E_{i+1} .

An important problem that needs to be addressed for all the steps above is load imbalance. Since the degree distribution on the original graph can be skewed and becomes more skewed for the coarsened graphs, a static vertex-to-thread assignment can reduce the performance. Hence *GOSH* uses a dynamic scheduling strategy, which uses small batch sizes for all the steps above.

3.3 Handling large graphs

One of the strongest points of *GOSH* is the ability to quickly generate a high-quality embedding of a large-scale graph on a single GPU. Here we present the techniques used when the graph and the embedding matrix do not fit in the GPU memory. The base algorithm for *GOSH* requires storing $d \times |V|$ and (|V|+1)+|E| entries for the matrix and the graph, respectively, for a graph G = (V, E). For large graphs with millions of vertices, a single GPU is unable to store this data.

We mitigate the bottleneck of storing \mathbf{M}_i on the GPU by using a partitioning schema similar to [8, 23], in which \mathbf{M}_i is partitioned and embedding is carried out on the sub-matrices instead of the entirety of \mathbf{M}_i . Formally, we partition V_i into K_i disjoint subsets of vertices $\mathcal{V}_i = \{V_i^0, V_i^1, \dots, V_i^{K_i-1}\}$. Let $\mathcal{P}_i = \{\mathbf{M}_i^0, \mathbf{M}_i^1, \dots, \mathbf{M}_i^{K_i-1}\}$ be the sub-matrices of \mathbf{M}_i corresponding to the vertex sets in \mathcal{V}_i . With partitioning, embedding G_i becomes the process of moving the sub-matrices in \mathcal{P}_i to the GPU, carrying out the training on these parts, and switching them out for the next sub-matrices, and so on.

In order to carry out the embedding correctly, all possible negative samples, chosen from $V_i \times V_i$, must be able to be processed. To do this, *GOSH* handles the embedding in rotations. During a rotation there will always be a point in time when \mathbf{M}_i^j and \mathbf{M}_i^k are together in the GPU for all $0 \le j < k < K$. When this happens, *B* positive and $B \times n_s$ negative samples are chosen from V_i^j (or V_i^k) for every vertex in V_i^k (or V_i^j). This way, in each rotation, we run a total of at most $B \times K_i$ updates on every vertex, which makes a full rotation (almost) equivalent to $B \times K_i$ epochs. We use the term *almost* since a vertex $v \in V_i^j$ may not have a neighbor in V_i^k . In this case, no positive updates are performed for v when V_i^j and V_i^k are on the device. Hence, running $\frac{e_i}{B \times K_i}$ rotations is (almost) equivalent to running e_i epochs for the embedding. We set B = 5 as the default value in *GosH* and experiment with different values to see its impact on embedding quality and performance.

Although partitioning the embedding matrix solves the first memory bottleneck, storing G_i on the GPU can still be problematic since this will leave less space for the sub-matrices. This is why we opt not to store G_i on the GPU. The positive samples are chosen on the host and only when required, they are sent to the GPU. Negative samples, on the other hand, are still generated on the GPU: the kernel for the parts (V_i^j, V_i^k) draws the negative samples for vertices in V_i^j randomly from V_i^k and vice versa for vertices in V_i^k .

3.3.1 Minimizing the data movements: Since the embedding is performed on pairs of sub-matrices, the rotation order in which we process the pairs is important to minimize the data movement operations. We follow an order resembling the *inside-out* order proposed in [8] which formally defines the part pairs as $(V_i^{a_0}, V_i^{b_0}), (V_i^{a_1}, V_i^{b_1}), \dots, (V_i^{a_\ell}, V_i^{b_\ell})$ where $\ell = \frac{K_i(K_i+1)}{2}$ and

$$(V_i^{a_j}, V_i^{b_j}) = \begin{cases} (V_i^0, V_i^0) & j = 0\\ (V_i^{a_{j-1}}, V_i^{b_{j-1}+1}) & j > 0 \text{ and } a_{j-1} > b_{j-1}\\ (V_i^{a_{j-1}+1}, V_i^0) & a_{j-1} = b_{j-1} \end{cases}$$

3.3.2 Choosing the sub-matrices and samples to be stored: Let P_{GPU} be the number of sub-matrices stored on the GPU at a time. Since we require every sub-matrix pair to exist on the GPU together during a single rotation, the smallest acceptable value is 2. However, $P_{GPU} = 2$ means that there will be time instances where all the kernels processing the current sub-matrices finish and a new kernel cannot start until a new sub-matrix is copied to the GPU. This leaves the GPU idle during the copy operation. On the other hand, using $P_{GPU} > 2$ occupies more space but allows an overlap of data transfers with kernel executions. For instance, assume M_i^1 , M_i^2 and M_i^4 are on GPU and the three upcoming kernels are $(V_i^4, V_i^1), (V_i^4, V_i^2)$ and (V_i^4, V_i^3) . The first two kernels are dispatched and after the first finishes, while the second is running, \mathbf{M}_{i}^{1} is replaced with \mathbf{M}_{i}^{3} , thus hiding the latency. A large P_{GPU} increases the amount of overlap. However, it also consumes more space on the GPU and increases K_i , i.e., the number of sets in \mathcal{V}_i . This leads to a rotation containing more kernels, i.e., pairs to be processed. For this reason, we set P_{GPU} = 3 to both hide the latency and occupy less GPU memory.

Since we do not keep the large graphs on GPU memory and draw positive samples on the CPU, these samples must also be transferred to the GPU for each kernel. However, if all these samples are transferred at once, similar to above, K_i increases and the performance decreases. To solve this issue, we only keep samples for S_{GPU} pairs on the GPU and dynamically replace a pool once it is consumed. We set $S_{GPU} = 4$ as we've experimentally found it to be an adequate value for all our graphs.

3.3.3 Implementation details: Embedding a large graph G_i requires an orchestrated execution of multiple tasks on the host and the device. *GOSH* coordinates the following tasks by single host thread:

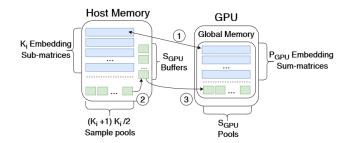


Figure 2: Memory model of large graphs algorithm embedding graph G_i . 1) Embedding sub-matrices are copied between the host and GPU as needed, 2) When sample pool $S_i^{j,k}$ is ready, it is copied to an empty buffer. 3) When a sample pool on the GPU is used up, it is replaced by the next sample pool from the buffer.

- (1) The main thread dispatches the embedding kernels to the GPU, as well as moves the sub-matrices forth and back between the host and GPU. Multiple GPU streams are used to allow for multiple kernel dispatches at once to maximize the utilization.
- (2) The SampleManager thread performs (positive) sampling into pools. When necessary, SampleManager creates a team of threads to generate samples for a single sample pool. Once a pool is ready to be sent to the GPU, it is kept in a buffer.
- (3) PoolManager dispatches the sample pools to the GPU. Once a sample pool is used up on the GPU, and becomes free to be overwritten, PoolManager dispatches a ready pool to the GPU.

Coordination among these threads is provided through condition variables. A high-level overview of the large graph embedding process is shown in Figure 2 and its pseudocode is given in Algorithm 5.

In Line 1 of Algorithm 5, we compute K_i and the number of rotations e^i . Line 2 initializes an array *GPUState* of size P_{GPU} which keeps track of embedding sub-matrices currently stored on the GPU. *GPUState*[j] = k means that bin j on the GPU currently holds M_i^k where an entry -1 indicates that the bin j is empty. At the beginning, the first P_{GPU} sub-matrices are copied to the GPU (lines 3–4) by calling the function SWITCHSUBMATRICES (j, k) which copies M_i^j out of the GPU, replaces it with M_i^k , and returns the new *GPUState*. Afterwards, the PoolManager and SampleManager threads are started and the main thread starts to perform the embedding rotations. Lines 7–13 run the main embedding loop.

When the sub-matrices \mathbf{M}_{i}^{m} , \mathbf{M}_{i}^{s} and the sample pool $S_{i}^{m,s}$ are ready, the function EMBEDDINGKERNEL (\mathbf{M}_{i}^{m} , \mathbf{M}_{s}^{s} , n_{s} , lr) runs the embedding kernel on the sub-matrices pair (\mathbf{M}_{i}^{j} , \mathbf{M}_{s}^{k}) using n_{s} negative samples and learning rate lr. Finally, the function NEXTSUB-MATRIX (*GPUState*, a, b) will determine the next sub-matrix to be switched into the GPU after running EMBEDDINGKERNEL (\mathbf{M}_{i}^{j} , \mathbf{M}_{i}^{k} , n_{s} , lr) given *GPUState*.

4 EXPERIMENTS

We will first explain the ML pipeline we used to evaluate embeddings and to compute AUCROC (Area Under the Receiver Operating GOSH: Embedding Big Graphs on Small Hardware

Algorithm 5: LARGEGRAPHGPU	
Data: G_i , M_i , n_s , lr , e_i , P_{GPU} , S_{GPU} , B	
Result: M _i	
1 $e' \leftarrow \frac{e_i}{B \times K_i}, K_i \leftarrow \text{GetEmbeddingPartInfo}(G_i)$	
$2 \ GPUState[0: P_{GPU} - 1] \leftarrow \{-1, -1, \dots, -1\}$	
3 for $i \leftarrow 0$ to $P_{GPU} - 1$ do	
$4 \qquad \qquad GPUState \leftarrow SwitchSubMatrices (-1, i)$	
5 THREAD(SampleManager, K_i , e' , S_{GPU})	
6 THREAD(PoolManager, K_i , e' , S_{GPU})	
7 for <i>r</i> from 1 to e' do	
s for m from 0 to $K_i - 1$ do	
9 for s from 0 to m do	
Wait for \mathbf{M}_{i}^{m} , \mathbf{M}_{i}^{s} and $S_{i}^{m,s}$ to be on GPU	
11 EMBEDDINGKERNEL $(\mathbf{M}_{i}^{m}, \mathbf{M}_{i}^{s}, n_{s}, lr)$	
12 $nextSM \leftarrow NextSubMatrix (GPUState, m,$	s)
13 GPUState ← SwitchSubMatrices (s, nextS	<i>5M</i>)

Characteristics) scores. Then the data-sets will be summarized and the state-of-the-art tools used to evaluate the performance of *GosH* will be listed. Lastly, the results will be given.

4.1 Evaluation with link-prediction pipeline

We evaluate the embedding quality of GOSH, VERSE, MILE, and GRAPHVITE with link prediction, which is one of the most common ML tasks that embedding algorithms are evaluated by [6, 8, 22, 23]. First, the input graph G is split into train and test sub-graphs as $G_{train} = (V_{train}, E_{train})$ and $G_{test} = (V_{test}, E_{test})$ respectively. G_{train} contains 80% of the edges of G, where G_{test} contains the remaining 20%. Then, we remove all the isolated vertices from G_{train} and also all (u, v) edges from G_{test} , where u or v is not in G_{train} . This guarantees that $V_{test} \subseteq V_{train}$. Next, we execute the tools to generate embeddings of G_{train} . Finally, we employ a Logistic Regression model which uses the embeddings generated in the previous step to predict the existence of edges in G_{test} . For medium scale graphs, we used the LogisticRegression module from scikit-learn. However, logistic regression becomes too expensive for large-scale graphs. Thus, for such graphs, we use the SGDClassifier module from scikit-learn with a logistic regression solver.

For the prediction pipeline, we create two matrices, \mathbf{R}_{train} , and \mathbf{R}_{test} . Each vector $\mathbf{R}_{train}[i]$ represents either a positive or a negative sample, and we obtain these vectors by doing element-wise multiplication of two vectors from \mathbf{M}_0 , corresponding to two vertices in the graph. \mathbf{R}_{train} includes all the edges in G_{train} as positive samples. Moreover, we generate $|E_{train}|$ number of negative samples from $(V_{train} \times V_{train}) \setminus E_{train}$ and add them as vectors to \mathbf{R}_{train} to make a balanced training set for the logistic regression classifier. In addition to d values obtained via element-wise multiplications, for \mathbf{R}_{train} , a label representing a positive or negative sample is concatenated to the end of the vector. Hence, the length of each \mathbf{R}_{train} vector is d + 1. We create \mathbf{R}_{test} in a similar fashion by using G_{test} instead of G_{train} as the source of the samples. We first train the logistic regression model using \mathbf{R}_{train} , and then test the

ICPP '20, August 17-20, 2020, Edmonton, AB, Canada

Table 2: Normal and large graphs used in the experiments.

Graph	$ \mathbf{V} $	E	Density
com-dblp[9]	317,080	1,049,866	3.31
com-amazon [9]	334,863	925,872	2.76
youtube [13]	1,138,499	4,945,382	4.34
soc-pokec [9]	1,632,803	30,622,564	18.75
wiki-topcats[9]	1,791,489	28,511,807	15.92
com-orkut[9]	3,072,441	117,185,083	38.14
com-1j[9]	3,997,962	34,681,189	8.67
soc-LiveJournal[9]	4,847,571	68,993,773	14.23
hyperlink2012[12]	39,497,204	623,056,313	15.77
soc-sinaweibo[18]	58,655,849	261,321,071	4.46
twitter_rv[18]	41,652,230	1,468,365,182	35.25
com-friendster[9]	65,608,366	1,806,067,135	27.53

validity of the model with \mathbf{R}_{test} . Finally, we report the *AUCROC* score obtained from the test set [4].

4.2 Datasets used for the experiments

We use various graphs in the evaluation process to cover many structural variations and to evaluate the tools in terms of performance and quality as fairly and thoroughly as possible. The graphs differ in terms of their origin, the number of vertices, and density. The properties of these graphs are given in Table 2. The mediumscale graphs, with less than 10M vertices, and large-scale ones are separated in the table.

4.3 State-of-the art tools used for evaluation

To evaluate the performance and the quality of *GOSH*, we use the results of the following state-of-the-art tools as a baseline.

VERSE: is a recent multi-core graph embedding tool [22]. It can employ different vertex-similarity measures including PPR, adjacency lists, and SimRank. We use the PPR similarity measure and $\alpha = 0.85$ as recommended by the authors. For *VERSE*, we set the epoch number to e = 600, 1000, and 1400, use a learning rate of lr = 0.0025 and report the best AUCROC. Larger learning rates produce worse results.

GRAPHVITE: is a state-of-the-art, fast multi-GPU graph embedding tool. However, according to [23], the algorithm cannot embed graphs with |V| > 12,000,000 on a single GPU. We use the default values for the hyperparameters as recommended by the authors and LINE is chosen as the base embedding method. As for the number of epochs, we use two settings; a fast setting with e = 600 epochs, and a slow setting with e = 1000 epochs.

MILE: performs embedding by coarsening a graph into multiple levels similar to *GOSH* [10]. It trains the smallest level and refines the embeddings up the coarsening levels. However, unlike *GOSH*, *MILE* uses a neural network to project the coarsened graph embedding to that of the original graph. We use the following parameters for the model: DEEPWALK as a base embedding method, MD-GCN as a refinement method, 8 levels of coarsening, and a learning rate of lr = 0.001. As for the epochs used during training, we note that *MILE* does not allow the number of epochs to be configured. Hence, that decision was left to the model itself.

For *GOSH*, we use three configurations: fast, normal and slow, with parameters given in Table 3. The configurations differ in terms

Table 3: GOSH configurations, fast, normal and small for medium-scale and large-scale graphs. A version with no coarsening is also used in the experiments.

Configuration	p	lr	e _{normal}	e _{large}
Fast	0.1	0.050	600	100
Normal	0.3	0.035	1000	200
Slow	0.5	0.025	1400	300
No coarsening	-	0.045	1000	200

of the number of epochs, smoothing ratio and learning rate. Compared to *GosH*-slow, *GosH*-fast uses a smaller p and a larger lr to compensate for the lesser number of epochs on the original graph with faster learning. Furthermore, we include in the experiments a version of *GosH* which does not perform coarsening. This configuration spends all of the epochs on the original graph. In addition to these differences, for medium-scale graphs, a larger number of epochs is used for each configuration compared to large-scale graphs.

For the experiments with *GOSH* and *VERSE*, we define a single epoch as sampling |E| target vertices. We do so to match the definition of an epoch given by *GRAPHVITE* [23] for the fairness of the experiments. With this definition, using fewer epochs for large-scale graphs makes more sense since a single epoch implies billions of samples and updates for such graphs, whereas for medium-scale graphs this number is in the order of tens of millions.

All the experiments run on a single machine with 2 sockets, each with 8 Intel E5-2620 v4 CPU cores running at 2.10GHz with two hyper-threads per core (32 logical cores in total), and 198GB RAM. To avoid the effects of hyper-threading, we only use 16 threads for parallel executions. The GPU experiments use a single Titan X Pascal GPU with 12GB of memory. The server has Ubuntu 4.4.0-159 as the operating system. All the CPU codes are compiled with gcc 7.3.0 with -03 as the optimization parameter. For CPU parallelization, OpenMP multithreading is used in general. Only for large graphs, a hybrid implementation with OpenMP and C++11 threading is employed. For GPU implementations and compilation, nvcc with CUDA 10.1 and optimization flag -03 are used. The GPUs are connected to the server via PCIe 3.0 x16. For GPU implementations, all the relevant data structures are stored on the device memory, unified memory is not used.

4.4 Experiments on coarsening performance

Table 4 provides the properties of the coarsenings obtained from the sequential and parallel coarsening algorithms with $\tau = 32$ threads. As the results show, parallel coarsening reaches a similar number of levels and the graphs at the last-level are of similar sizes. Hence, there is a negligible difference regarding the quality of graphs generated by the two algorithms. Only for soc-sinaweibo, there is a one-level difference for which $|V_{D-1}|$ also has a difference of 142 vertices.

With a similar coarsening quality, the parallel algorithm is 5– 10× faster compared to the sequential counterpart. As described in Section 3.2.2, the time complexity is O(|V| + |E|) and in practice, |E|dominates the workload. Although there are other parameters, the variation in the speedups is in concordance with the variation in the number of edges. For instance, soc-sinaweibo only has 200M edges and yields the smallest speedup value of $5.8 \times$. On the other hand, the largest speedup $10.5 \times$ is obtained for com-friendster, which is the largest in our data-set with 1.8B edges.

Table 4: Execution times, the number of levels and the size of the last-level graphs for sequential and parallel coarsening with $\tau = 32$ threads for the large-scale graphs. The results are the average of 5 runs.

Graph	τ	Time (s)	Speedup	D	$ V_{D-1} $
human link 2012	1	365.49	-	8	2411
hyperlink2012	32	45.36	8.06×	8	2385
soc-sinaweibo	1	135.92	-	10	272
SOC-SINAWEIDO	32	23.54	5.77×	9	414
twitter_rv	1	629.20	-	12	541
twitter_iv	32	77.77	8.09×	12	432
com-friendster	1	2468.52	-	10	1164
com-ri ienuster	32	235.38	$10.49 \times$	10	1158

4.4.1 GOSH vS MILE. In Table 5, we show a brief comparison of MILE and GOSH with 16 threads on the graph com-orkut. Since MILE does not have a stopping criterion for coarsening, we used the same amount of coarsening levels for both algorithms. While coarsening a graph of 3 million vertices and 100 million edges, GOSH is 264 times faster than MILE. Moreover, GOSH is a lot more efficient regarding the number of vertices obtained at each level. For instance, in 8 levels GOSH shrinks com-orkut to only 230 vertices, while MILE shrinks it to 12062 vertices. This is important since the training time is affected by the number of vertices at each level.

4.5 Experiments on handling large graphs

Figure 3 shows the effect of adjusting the batch size *B* for largegraph embedding. The top figure provides the execution time and the bottom figure provides the AUCROC scores. We can see the trade-off between performance and quality while increasing *B*. The execution time decreases since the number of embedding rounds is reduced. However, the quality also decreases since increasing *B* results in increasing the number of updates being carried out on a subset of the graph *in isolation* from the rest of the embedding process. To be as efficient as possible and not to decrease the accuracy significantly, we use B = 5 as the default value for *GosH*.

Table 5: *MILE* vs *GOSH* coarsening on com-orkut. A parallel coarsening with $\tau = 16$ threads is used for *GOSH*.

	i	Time (s)	$ V_i $		i	Time (s)	$ V_i $
	0	-	3056838		0	-	3056838
	1	249.77	1535168		1	4.44	975132
	2	237.39	768804		2	1.23	213707
	3	184.72	384752		3	0.62	46667
MILE	4	151.24	192507	Gosh	4	0.16	8084
N	5	139.23	96308	0	5	0.03	2000
	6	128.47	48183		6	0.01	701
	7	117.75	24107		7	< 0.01	375
	8	99.73	12062		8	< 0.01	275
	Total	1308.31	-		Total	6.60	-

Table 6: Link prediction results on medium-scale graphs. Every data-point is the average of 15 results. Verse and GOSH uses $\tau = 16$ threads. Mile is a sequential tool. Both GRAPHVITE and GOSH uses the same GPU. The speedup values are computed based on the execution time of Verse.

Graph	Algorithm	Time (s)	Speedup	AUCROC(%)	Graph	Algorithm	Time (s)	Speedup	AUCROC(%)
	Verse	247.99	$1.00 \times$	97.82		Verse	216.18	$1.00 \times$	97.71
	Mile	136.65	1.81×	97.65	1	Mile	146.29	1.48×	98.14
	GRAPHVITE-fast	13.97	17.70×	97.80	1	GRAPHVITE-fast	12.45	17.36×	97.40
com-dblp	GRAPHVITE-slow	19.93	$12.40 \times$	98.08	com-amazon	GRAPHVITE-slow	16.84	$12.83 \times$	97.82
	Gosн-fast	0.72	344.43×	96.45	1	Gosн-fast	0.69	313.30×	97.20
	Gosн-normal	2.08	119.23×	97.38		Gosн-normal	1.88	$114.99 \times$	98.29
	GosH-slow	3.84	$64.58 \times$	97.63		GosH-slow	3.59	60.22×	98.43
	Gosh-NoCoarse	29.97	8.27×	93.31	1	Gosh-NoCoarse	24.60	8.79×	90.13
	Verse	12502.72	1.00×	98.86		Verse	45994.93	$1.00 \times$	98.65
	Mile	3948.62	3.17×	80.19		Mile	11904.31	3.86×	90.38
1 <i>-:</i>	GRAPHVITE-fast	373.58	33.47×	98.04		GRAPHVITE-fast	1246.38	36.90×	98.02
com-lj	GRAPHVITE-slow	644.43	$19.40 \times$	98.33	com-orkut	GRAPHVITE-slow	2199.25	$20.91 \times$	98.05
	Gosн-fast	16.27	768.45×	96.82		Gosн-fast	43.30	$1062.24 \times$	97.35
	Gosн-normal	55.01	$227.28 \times$	98.33		Gosн-normal	185.12	$248.46 \times$	97.63
	GosH-slow	153.72	81.33×	98.46		GosH-slow	487.33	94.38×	97.69
	Gosh-NoCoarse	675.25	18.52×	98.32		Gosh-NoCoarse	2301.89	19.98×	97.64
	Verse	8709.48	1.00×	99.31		Verse	1365.36	1.00×	98.04
	Mile	4953.68	1.76×	86.04	1	Mile	1328.62	1.03×	94.17
wiki-	GRAPHVITE-fast	310.47	28.05×	96.42	voutube	GRAPHVITE-fast	63.90	21.37×	97.07
topcats	GRAPHVITE-slow	544.06	$16.01 \times$	96.28	yourube	GRAPHVITE-slow	104.76	$13.03 \times$	97.45
	Gosн-fast	11.34	768.03×	98.13	1	Gosн-fast	2.76	494.70×	96.16
	Gosн-normal	40.76	$213.68 \times$	98.33		Gosн-normal	7.15	$190.96 \times$	97.78
	GosH-slow	93.86	92.79×	98.50		GosH-slow	15.32	89.12×	97.93
	Gosh-NoCoarse	549.65	15.85×	98.51	1	Gosн-NoCoarse	158.60	8.61×	97.16
	Verse	9182.53	1.00×	98.32		Verse	14965.76	$1.00 \times$	97.61
	Mile	2848.78	3.22×	85.75	1	Mile	6210.58	2.41×	80.84
	GRAPHVITE-fast	370.73	$24.77 \times$	97.42	soc-	GRAPHVITE-fast	745.33	20.08×	99.23
soc-pokec	GRAPHVITE-slow	607.07	15.13×	97.37	LiveJournal	GRAPHVITE-slow	1209.95	$12.37 \times$	99.31
	Gosн-fast	16.34	561.97×	96.34	1	Gosн-fast	29.74	503.22×	98.58
	Gosн-normal	54.66	167.99×	96.49		Gosн-normal	112.72	$132.77 \times$	98.87
	GosH-slow	131.06	70.06×	96.67		GosH-slow	183.64	81.50×	98.76
	Gosh-NoCoarse	598.95	15.33×	97.28	1	Gosн-NoCoarse	1348.74	11.10×	98.88

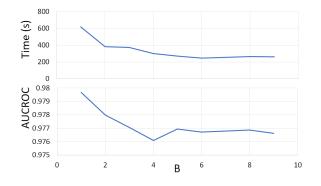


Figure 3: Running large-graph embedding on hyperlink with different *B* values.

4.6 Experiments on embedding quality

Tables 6 and 7 provide the execution times and AUCROC scores of the tools evaluated in this work on medium-scale and large-scale graphs, respectively. The parameters for the tools are given in Section 4.3 (see Table 3 for *GosH* configurations). The first observation is that coarsening does not have a significant negative effect on the quality of the embedding. While *GosH* performs worse on some

medium-scale graphs with coarsening, for others, the scores are approximately the same or even better. Since all of the epochs are reserved for the original graph in the non-coarsened version, we expect the results of this configuration to be more fine-tuned. However, the data shows that training in the coarser levels may have a more prominent effect than training more on the original graph.

In addition to *GOSH* configurations, we use *GRAPHVITE*, *MILE*, and *VERSE* on medium-scale graphs. The results are given in Table 6. To evaluate the runtime performance of the tools, we use the execution time of *VERSE* as the baseline and present the speedups by each tool. From these experiments, we have the following observations:

• *GOSH*-fast is an ultra-fast solution that produces very accurate embeddings at a fraction of the time compared to all the systems under evaluation. It can achieve a speedup over *VERSE* of up to three orders of magnitude and an average of 600× with a maximum loss in AUCROC of 2% and an average loss of 1.16%. When compared to *MILE*, it is superior in terms of AUCROC in six out of eight graphs while being at least two orders of magnitude faster. As for *GRAPHVITE*, we see that, at an average loss in AUCROC of 0.54%, *GRAPHVITE* can achieve an average speedup of 23.44×.

- *Gosh*-normal demonstrates the speed/quality trade-off of *Gosh* and its flexibility. Switching from *Gosh*-fast to *Gosh*-normal results in an average AUCROC increase of 0.76% while only reducing the speed on average by a factor of 3×.
- The flexibility is demonstrated further by *GosH*-slow whose accuracy becomes close to the best tool for every graph. Compared to *VERSE*, this configuration has an average loss of 0.24% in AUCROC, but still has an average speedup of 79.24×.
- To compare *Gosh* with the state-of-the-art GPU implementation *GRAPHVITE*, we used the best AUCROCs of the tools. For 4/8 graphs, *Gosh* configurations produce better AUCROC compared to *GRAPHVITE* configurations. The values are similar; on average, *Gosh* achieves 0.16% higher AUCROCs than *GRAPHVITE*. However, *Gosh* is 5.2× faster than *GRAPHVITE* on average.

4.6.1 Large-scale graphs. The results of the experiments for large-scale graphs can be seen in Table 7. We observe the following:

GRAPHVITE results are not reported since, for all the large-scale graphs, the executable runs out of CPU memory on our machine. We find that *GRAPHVITE* on hyperlink2012 is reported to achieve 94.3% link-prediction AUCROC after an embedding for 5.36 hours using four Tesla P100s GPUs [23]. *GOSH*-normal achieves an AUCROC of 97.20% after an embedding taking only 0.2 hours using a single Titan X GPU (26.8× speedup). It is also reported that *GRAPHVITE* takes 20.3 hours on com-friendster [23] where *GOSH*-normal requires only 0.76 hours (26.7× speedup).

MILE cannot embed hyperlink2012 and soc-sinaweibo before the 12 hour timeout. Furthermore, the executable failed to run on the other two graphs due to insufficient memory.

Verse timed out for 3 of the 4 graphs, as shown in Table 7. However, it performed the embedding on soc-sinaweibo successfully. Compared to *Gosh*-slow, it scores a 0.52% higher AUCROC. On the other hand, *Gosh*-slow achieves a 26× speedup over *Verse*.

4.7 Experiments on smaller dimensions

We analyzed the performance of *GOSH* when multiple vertices are assigned to a single warp, where *d* is small. The results on com-orkut and soc-LiveJournal are given in Table 8. Without small-dimension technique (SM), *GOSH* takes approximately the same time for d = 8, 16 and 32 where $4 \times$ and $2 \times$ less work is performed for d = 8 and 16. With SM, we observe 2.63× and 1.84× speedups for d = 8 and 16, respectively. Moreover, for soc-LiveJournal, we obtain 2.70× and 1.85× speedups for d = 8and d = 16, respectively. As expected, with or without SM, d = 32timings are almost the same.

4.8 Speedup breakdown

For a more detailed analysis of performance improvements, we run intermediate versions of *GosH* and report the speedup over 16-thread CPU implementation. The experiments are conducted with six graphs; two large-scale graphs (com-friendster, and hyperlink2012), and four medium-scale graphs. We did not run the GPU implementations that are not using coarsening on the large-scale graphs as they take a long amount of time. The results are presented in Figure 4.

Table 7: Link prediction results on large graphs. Every datapoint is the average of 6 results. *GRAPHVITE* and *MILE* fail to embed any of the graphs due to excessive memory usage or an execution time larger than 12 hours. $\tau = 16$ threads used for both *VERSE* and *GOSH*.

				AUC
Graph	Algorithm	Time (s)	Speedup	ROC (%)
	Verse	Timeout	-	-
human link 2012	Gosн-fast	201.02	-	87.60
hyperlink2012	Gosн-normal	724.09	-	97.20
	GosH-slow	1676.93	-	98.00
	Verse	20397.79	$1.00 \times$	99.89
soc-sinaweibo	Gosн-fast	48.88	417.30×	70.27
soc-sinaweibo	Gosн-normal	352.86	57.81×	97.00
	GosH-slow	759.85	$26.84 \times$	99.37
	Verse	Timeout	-	-
tuittan nu	Gosн-fast	261.08	-	91.78
twitter_rv	Gosн-normal	994.46	-	97.36
	GosH-slow	2128.70	-	98.50
	Verse	Timeout	-	-
com-friendster	Gosн-fast	680.33	-	85.17
com-11 tends ter	Gosн-normal	2720.82	-	93.40
	GOSH-slow	5000.96	-	94.98

Table 8: Performance of GOSH with (SM = Yes) & without (SM = No) small-dimension embedding and $\tau = 16$ threads.

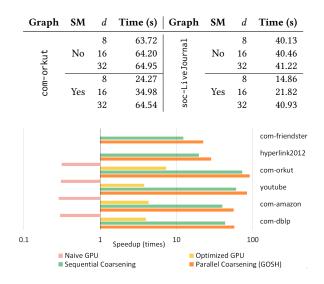


Figure 4: The speedups obtained from running intermediate versions of *GOSH* compared to our multi-core CPU implementation with 16 threads.

The first *GOSH* version is the *Naive GPU* implementation that results in an average slowdown of 3.3×. The *Optimized GPU* version leverages architecture-specific optimizations to reduce memory access overhead. That is, global memory is organized to have coalesced accesses, and shared memory is utilized to reduce the number of global memory accesses. This version is 5.4× faster than the 16-thread one. These two versions do not use coarsening.

The next version employs *Sequential Coarsening*, as well as all the GPU optimizations from the previous one. This *GOSH* version scores an average speedup of 45× over the CPU version, while maintaining the embedding quality as shown in Table 6. This is due to the cumulative nature of the updates on the coarsened graphs, where a single update on a super vertex is propagated to all the vertices it contains.

The *Parallel Coarsening* version, which is the final *GOSH*, further improves the performance. As discussed in Section 4.4, the performance difference between *Parallel Coarsening* and *Sequential Coarsening* is expected to be more for larger graphs. For instance, on com-friendster, sequential and parallel coarsening phases take 2468.52 and 235.38 seconds, respectively (Table 4). On the same graph, the total run-time of *GOSH*-normal is 2720.82 seconds (Table 7). In other words, parallel coarsening results in an 80% improvement on performance.

5 RELATED WORK

There are various approaches proposed for embedding graphs. A survey on these techniques can be found in [5]. For instance, in matrix factorization based embedding, the matrix representing the relationship between vertices in the graph is factorized [1, 2, 16, 19]. Another approach in the literature is the sampling-based embedding [6, 17, 21, 22] in which the samples are drawn from the graph and used to train a single-layer neural network. Different embedding algorithms use different sampling strategies, most notable of which are random walks [6, 17]. Each algorithm in the literature tries to capture the structural and role/class information based on a similarity measure and/or a sampling strategy. There also have been attempts [16, 22] for a more generalized embedding process.

Graph embedding is an expensive task and hard to perform without high-performance hardware. Graph coarsening [3, 10], as well as distributed system approaches [8, 15, 20] have been previously used to tackle this issue. However, these methods do not fully utilize a specialized, now ubiquitous piece of hardware, GPU. The literature does not usually focus on the performance of coarsening since, on CPUs, embedding is slow and coarsening time is negligible. However, this is not the same for GPUs. Furthermore, even state-of-the-art embedding tools are using coarsening schemes that cannot shrink the graphs well.

There have been attempts to make the embeddings faster by utilizing GPUs; *GRAPHVITE* generates samples on the host device and performs the embedding on the GPU [23]. However, when the total GPU memory is not capable of storing the embedding matrix, the tool cannot perform the embedding. To the best of our knowledge, there is no sampling-based graph embedding tool in the literature which is designed for memory restricted but powerful GPUs. *GosH* tries to utilize the power of GPUs by applying coarsening and using a judiciously orchestrated CPU-GPU parallelism.

6 CONCLUSION AND FUTURE WORK

In this paper, we introduce a high-quality, fast graph embedding approach that utilizes CPU and GPU at the same time. The tool can embed any graph by employing a partitioning schema along with dynamic on-CPU sampling. In addition to this, we provide optimization techniques to minimize GPU idling and maximize GPU utilization during embedding. Furthermore, a parallel coarsening algorithm, which outperforms the state-of-the-art coarsening techniques both in terms of efficiency and speed, is proposed. We finetuned the coarsening approach to produce high-quality embeddings at a fraction of the time spent by the state-of-the-art. Our experiments demonstrate the effectiveness of *GOSH* on a wide variety of graphs. In the future, we are planning to make *GOSH* publicly available with easy-to-use interfaces for widely used software such as Matlab and scikit-learn. Furthermore, we will extend our work for other ML tasks such as classification and anomaly detection.

REFERENCES

- M. Belkin and P. Niyogi. 2001. Laplacian Eigenmaps and Spectral Techniques for Embedding and Clustering. In Proc. 14th Int. Conf. on Neural Information Processing Systems: Natural and Synthetic (British Columbia, Canada) (NIPS'01). MIT Press, Cambridge, MA, USA, 585–591.
- [2] S. Cao, W. Lu, and Q. Xu. 2015. GraRep: Learning Graph Representations with Global Structural Information. In Proc. 24th ACM Int. Conf. on Info. and Knowledge Management (Melbourne, Australia) (CIKM '15). ACM, NY, USA, 891–900.
- [3] H. Chen, B. Perozzi, Y. Hu, and S. Skiena. 2017. HARP: Hierarchical Representation Learning for Networks. arXiv:1706.07845 [cs.SI]
- [4] T. Fawcett. 2006. An Introduction to ROC Analysis. Pattern Recogn. Lett. 27, 8 (June 2006), 861–874. https://doi.org/10.1016/j.patrec.2005.10.010
- [5] P. Goyal and E. Ferrara. 2018. Graph Embedding Techniques, Applications, and Performance: A Survey. Knowl. Based Syst. 151 (2018), 78–94.
- [6] A. Grover and J. Leskovec. 2016. node2vec: Scalable Feature Learning for Networks. arXiv:1607.00653 [cs.SI]
- [7] R. Hu, C. C. Aggarwal, S. Ma, and J. Huai. 2016. An embedding approach to anomaly detection. In 2016 IEEE 32nd Int. Conf. on Data Eng. (ICDE). 385–396.
- [8] A. Lerer, L. Wu, J. Shen, T. Lacroix, L. Wehrstedt, A. Bose, and A. Peysakhovich. 2019. PyTorch-BigGraph: A Large-scale Graph Embedding System. arXiv:1903.12287 [cs.LG]
- [9] Jure Leskovec and Andrej Krevl. 2014. SNAP Datasets: Stanford Large Network Dataset Collection. http://snap.stanford.edu/data.
- [10] J. Liang, S. Gurukar, and S. Parthasarathy. 2018. MILE: A Multi-Level Framework for Scalable Graph Embedding. arXiv:1802.09612 [cs.AI]
- [11] D. Liben-Nowell and J. Kleinberg. 2003. The Link Prediction Problem for Social Networks. In Proc. 12th Int. Conf. on Information and Knowledge Management (New Orleans, LA, USA) (CIKM '03). ACM, NY, USA, 556–559.
- [12] R. Meusel. 2015. The Graph Structure in the Web Analyzed on Different Aggregation Levels. *Journal of Web Science* 1 (08 2015), 33–47.
- [13] A. Mislove, M. Marcon, K. P. Gummadi, P. Druschel, and B. Bhattacharjee. 2007. Measurement and Analysis of Online Social Networks. In *Proceedings of the 7th* ACM SIGCOMM Conference on Internet Measurement (San Diego, California, USA) (IMC '07). ACM, New York, NY, USA, 29–42.
- [14] F. Niu, B. Recht, C. Re, and Stephen J. Wright. 2011. HOGWILD! A Lock-Free Approach to Parallelizing Stochastic Gradient Descent. In Proc. 24th Int. Conf. on Neural Information Processing Systems (Granada, Spain) (NIPS'11). Curran Associates Inc., NY, USA, 693–701.
- [15] E. Ordentlich, L. Yang, A. Feng, P. Cnudde, M. Grbovic, N. Djuric, V. Radosavljevic, and Gavin Owens. 2016. Network-efficient distributed word2vec training system for large vocabularies. In Proc. 25th ACM Int. Conf. on Information and Knowledge Management. ACM, xx, 1139–1148.
- [16] M. Ou, P. Cui, J. Pei, Z. Zhang, and W. Zhu. 2016. Asymmetric Transitivity Preserving Graph Embedding. In Proc. 22nd Int. Conf. on Knowledge Discovery and Data Mining (San Francisco, CA, USA) (KDD '16). ACM, NY, USA, 1105–1114.
- [17] B. Perozzi, R. Al-Rfou, and S. Skiena. 2014. DeepWalk: Online Learning of Social Representations. In Proc. 20th ACM SIGKDD Int. Conf. on Knowledge Discovery and Data Mining (NY, USA) (KDD '14). ACM, NY, USA, 701–710.
- [18] R. A. Rossi and N. K. Ahmed. 2015. The Network Data Repository with Interactive Graph Analytics and Visualization. In AAAI. http://networkrepository.com
- [19] S. T. Roweis and L. K. Saul. 2000. Nonlinear dimensionality reduction by locally linear embedding. science 290, 5500 (2000), 2323–2326.
- [20] N. Shazeer, R. Doherty, C. Evans, and Chris Waterson. 2016. Swivel: Improving Embeddings by Noticing What's Missing. arXiv:1602.02215 [cs.CL]
- [21] J. Tang, M. Qu, M. Wang, M. Zhang, J. Yan, and Q. Mei. 2015. LINE: Large-Scale Information Network Embedding. In Proc. 24th Int. Conf. on World Wide Web (Florence, Italy). IW3C2, 1067–1077.
- [22] A. Tsitsulin, D. Mottin, P. Karras, and E. Müller. 2018. VERSE: Versatile Graph Embeddings from Similarity Measures. In Proc. World Wide Web Conference (Lyon, France) (WWW '18). IW3C2, Republic and Canton of Geneva, CHE, 539–548.
- [23] Z. Zhu, S. Xu, J. Tang, and M. Qu. 2019. GraphVite: A High-Performance CPU-GPU Hybrid System for Node Embedding. In *The World Wide Web Conference* (CA, USA) (WWW '19). ACM, NY, USA, 2494–2504.