GL-Coarsener: A Graph representation learning framework to construct coarse grid hierarchy for AMG solvers

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In many numerical schemes, the computational complexity scales non-linearly with the problem size. Solving a linear system of equations using direct methods or most iterative methods is a typical example. Algebraic multi-grid (AMG) methods are numerical methods used to solve large linear systems of equations efficiently. One of the main differences between AMG methods is how the coarser grid is constructed from a given fine grid. There are two main classes of AMG methods; graph and aggregation based coarsening methods. Here we propose an aggregation-based coarsening framework leveraging graph representation learning and clustering algorithms. Our method introduces the power of machine learning into the AMG research field and opens a new perspective for future researches. The proposed method uses graph representation learning techniques to learn latent features of the graph obtained from the underlying matrix of coefficients. Using these extracted features, we generated a coarser grid from the fine grid. The proposed method is highly capable of parallel computations. Our experiments show that the proposed method’s efficiency in solving large systems is closely comparable with other aggregation-based methods, demonstrating the high capability of graph representation learning in designing multi-grid solvers.

Keywords: Algebraic Multi-Grid, Graph Representation Learning, Coarsening

1 INTRODUCTION

Many real-world problems are governed by partial differential equations (PDEs). For example, to predict the forces induced by airflow on a car or an airplane, Computational Fluid Dynamics (CFD) relies on the solution of non-linear Navier Stokes Equations (NSE). To model these problems, large complex meshes are constructed. After applying numerical methods, it results in a massive system of linear equations (order of million to billion) to be solved many times (order of thousand to million) during the simulation process [1].

The typical way to solve PDEs is to discretize the PDE to equations that involve a finite number of unknowns. This is usually achieved using Finite Differences Method (FDM),

Finite Volume Method (FVM), or Finite Element Method (FEM). At the heart of these processes is solving efficiently a linear systems of equations in the form of:

\[ Au = f \] (1)

where A is a sparse coefficient matrix resulted from the discretization of the original PDE which is called stiffness matrix in some cases.

There are many methods that could be used to solve systems of linear equations similar to Eq. 1. These methods could be sorted into two main categories: direct or iterative methods.

Direct methods like variable elimination techniques, row reduction techniques (e.g., Gaussian elimination), Cramer’s technique and inverse matrix solution will result in an exact (up to machine accuracy) solution. Direct methods have a typical time complexity of \(O(n^3)\) [2]. As the system’s size increases, it becomes computationally costly to use direct methods, which is the main reason they are not usually used for real-world engineering problems. Moreover, they usually destroy the original matrix’s sparsity, making it hard to keep on high-speed Random Access Memory (RAM).

Indirect (iterative) methods like Jacobi, Gauss-Seidel, and Successive Over-Relaxation (SOR) usually converge to an accurate enough approximation for the system [3]. Under the right condition, these iterative methods will rapidly damp the approximate solution’s high-frequency errors in a few steps -smoothing the approximate solution- but are ineffective when it comes to damping low-frequency errors.
Two important properties of the iterative methods are that they provide good approximations in manageable amounts of time and they do not destroy the sparsity of the coefficient matrix.

Multi-grid (MG) methods are a powerful class of iterative solvers that could efficiently solve discretized differential equations. As mentioned previously, iterative solvers (smoothers) like Jacobi are useful for damping high-frequency errors. Unfortunately, after a few iterations, their convergence rate decreases drastically and usually the slow convergence rate associated with the low-frequency errors dominates the error reduction rate. To address this issue, multi-grid methods introduce a hierarchy of coarser grids. With proper mapping (called prolongation) the low-frequency errors with respect to the fine grid are represented as high-frequency error relative to coarse grid; therefore the smoothers would keep their high rate of convergence on the coarse grid. As such, multi-grid methods can be regarded more as a strategy than stand-alone solvers [4].

A coarse grid is a lower resolution representation of the original fine grid. The key to success of multi-grid strategy is the fact that the low-frequency errors of the finer grid will become high frequency in the coarser grid [5].

The coarse grid problem could either be constructed from the original physics (Physical or Geometric Multi Grid) or constructed from the fine grid’s existing coefficient matrix (Algebraic Multi-grid, AMG). In this work, we focus on AMG. One of the main differences between different AMG methods is how they move from a fine grid to a coarser grid. When it comes to constructing the coarser grid from the fine grid, AMG methods fall into two main categories [6]:

1- Graph based AMG methods (e.g., Beck, Ruge-Stüben)
2- Aggregation based AMG methods (e.g., Vaněk, Adaptive Smoothed Aggregation (aSA))

This paper proposes GL-Coarsener framework, an aggregation-based AMG, for constructing the coarser grid linear system from that of the given fine grid leveraging the underlying connections in the fine grid’s graph.

GL-Coarsener consists of two main modules:

- Embedding module: The underlying fine grid is projected into a d-dimensional embedding space.
- Clustering module: The aggregates are constructed by applying clustering techniques on the embedding space obtained from the embedding module.

To the best of our knowledge, our work is the first aggregation based AMG that utilizes graph representation learning techniques to select aggregates intelligently.

The rest of the paper is organized as follows. In section 2 we briefly review the related works and researches done in AMG field. In section 3 the required preliminaries will be explained. We present our proposed method in section 4. Finally, in section 5 we compare the performance of our method with other available methods.

2 RELATED WORK

Algebraic multi-grid was first described in 1980s [7]. This method assumes no information is provided about the geometry of the underlying grid and takes the coefficient matrix (A) which could be obtained from the discretized PDE problem to construct the multilevel hierarchy. The earliest algebraic multi-grid methods are graph-based methods. By introducing some criteria to determine strongly connected nodes, graph-based methods label nodes as coarse or fine by taking into account the count of a node’s strong connections and the strength of connections.

A popular graph-based algorithm is Ruge-Stüben [8], introduced in 1981, this method and it’s refined versions are still widely used. Ruge-Stüben takes a threshold to distinguish between weak and strong connections; the nodes with more strong connections are selected to be coarse nodes. The prolongation operator is then constructed by considering the number of strong connections of each node. Later implementations of this method include P. Zaspel [9], which proposes a parallelized GPU implementation of Ruge-Stüben to improve the algorithm’s performance.

The Beck method is a simpler coarsening method which does not distinguish between strong and weak connections [10]. This results in less robustness, meaning that it cannot recover the usual multi-grid efficiency for non-smooth coefficient PDEs, but allows for an easier and less complex implementation. Beck method carries out the task of labelling nodes and constructs transfer operators by considering only the number of connections.

Aggregation based methods are a class of coarseners that differ from graph based methods in how the coarse grid is constructed. Aggregate methods make use of connection strength, but only to form neighborhoods of points. These neighborhoods are then taken as a unit while selecting the coarse grid [3]. The first aggregation method was introduced by Vaněk. The standard aggregation defines the strongly coupled neighborhood of a node i with threshold ε as follows:

\[ N_i(\epsilon) = \{ j \in \Lambda_h : |A_{ij}| \geq \epsilon \sqrt{|A_{ii}|A_{jj}} \} \]  

where \( \Lambda_h \) is the set of node indices in fine level adjacency matrix. These neighborhoods are used to form aggregates of nodes denoted by C. Once the aggregates are selected, the corresponding prolongation matrix is constructed using the cluster (aggregate) assigned to each node.

The preliminary prolongation matrix \( \hat{P} \) in standard aggregation is defined as the following:

\[ \hat{P}_{ij} = \begin{cases} 1, & i \in C_j; \\ 0, & otherwise. \end{cases} \]  

where i and j iterate over nodes and clusters respectively. This prolongation operator is used in this paper.

1Aggregation is used in two different contexts in this article. One refers to grouping nodes in AMG context and the other refers to accumulation of node features in graph learning algorithms.
Recent improvements on aggregation based methods include adaptive aggregation \cite{12}, and accelerated adaptive aggregation methods \cite{13}.

3 PRELIMINARIES

In this section, we first review the basics of AMG, then we describe the machine learning techniques used in this paper.

3.1 Algebraic Multi-grid (AMG)

It is well known that stationary iterative linear solvers (like Jacobi and Gauss-Seidel) cannot efficiently damp low-frequency errors, especially for large sparse symmetric positive definite (SPD) systems. Further analysis of iterative solvers has proven that this loss of convergence rate is related to the system’s smallest eigenvalues. To recover the convergence rate, algebraic multi-grid methods construct a hierarchy of operators to map the system of equations to a coarser system with a fewer number of unknowns. As is shown in Fig. 1 the low-frequency errors of the fine grid problem (related to lowest eigenvalues) are represented as high-frequency errors on the next coarse grid. Progressively constructing coarser grids, AMG methods will construct systems of equations with relative high eigenvalues; therefore, the iterative smoothers’ convergence rate is recovered on coarse grid and it could efficiently reduce the errors again.

As demonstrated in Fig. 1 AMG methods work in five main phases:

1- The approximate solution $v$ obtained from applying a few iterations of the smoother will be used to calculate the fine grid residual:

$$r = f - Av$$

$$= Au - Av$$

$$= A(u - v) = Ae$$

in which $f$ is the right-hand-side matrix of the original system (Eq. 1) and $e$ is the error involved in approximating $u$ with $v$.

2- A coarse grid is selected, and a restriction operator is constructed to map the coefficient matrix ($A_f$) from the fine grid to the coarse grid.

3- The residual Eq. 4 is solved on the coarse grid. The solution in this step is accelerated by recursive application of the multi-grid method until the coarsest grid is reached, for which obtaining an exact solution using direct methods would be cheap.

4- The third phase’s solution is interpolated back to the fine grid, usually using the restriction operator’s transpose.

5- The interpolated solution is used to modify the approximate solution $v$ to $v + e$. This correction will reduce low-frequency errors in $v$ for which the smoother had a low rate of convergence. Before and after each multi-grid iteration, a smoothing step is usually applied to the system of equations to damp the high-frequency errors. These steps are called pre-smoothing and post-smoothing. AMG algorithms are usually described as a recursive application of the two-grid method. Algorithm 1 explains a two-level AMG algorithm.

Algorithm 1 One iter. of two-level Algebraic Multi-grid

\begin{algorithm}
\caption{One iter. of two-level Algebraic Multi-grid}
\begin{algorithmic}
\State \textbf{Input:} $A_f, f_f$ \Comment{$A_f u_f = f_f$ is the fine-level system}
\State \textbf{Output:} Corrected $v_f$
\State 1: $r_f \leftarrow f_f - A_f v_f$
\State 2: Construct prolongation operator $P$
\State 3: $R \leftarrow P^T$
\State 4: $A_c \leftarrow R P$
\State 5: $r_c \leftarrow R r_f$
\State 6: Solve $A_c e_c = r_c$ recursively for $e_c$
\State 7: $e_f \leftarrow P r_c$
\State 8: return $v_f + e_f$
\end{algorithmic}
\end{algorithm}

3.2 Machine Learning

3.2.1 node2vec

Graph learning and feature representation are the main concepts behind the embedding module of our method. This would allow for accurate downstream machine learning tasks such as clustering.

Dimensionality reduction techniques for unsupervised feature learning such as Vazquez \cite{14} and Tenenbaum \cite{15} could be used in this work, but these methods show lower computational performance, and become increasingly more difficult when scaled to large graphs. The Skip-gram model \cite{16} uses neural network models to learn word feature vectors from huge data sets with billions of words. This algorithm is based on the hypothesis that similar words tend to be closer to each other. Moreover, words can have multiple degrees of similarity \cite{17}. The skip-gram model and the idea of feature representation was further extended to networks by DeepWalk algorithm \cite{18}; DeepWalk generates random-walks on nodes to analyze graphs and learn latent representations of vertices in a network.

This work is further developed by node2vec algorithm. The algorithm adopts a flexible parameter tuning for node sampling to learn richer representation in different networks \cite{19}.

One of the newer methods for representing graphs is using convolutional neural networks (CNN) \cite{20}. The basic idea is to slide a filter over the structure of the grid to learn representation of nodes. However, this approach makes the algorithm dependent on the structure of the grid therefore the training does not generalize to various formations of graphs. Graph convolutional networks (GCN), on the other hand, learn aggregations of a node’s neighbours to construct the node’s feature vector \cite{21}. Such methods are independent of the ordering of nodes and the structure.

\footnote{Usually a small number of iterations (1 to 5) of smoothing is sufficient}
Fig. 1. Illustration of a two-grid V-cycle

of the graph. This grants the embedder transductivity property, which allows for generation of node embeddings to previously unseen data. GraphSAGE algorithm [22] is a developed GCN variant, which trains a set of aggregator functions that learn to aggregate feature information from a node’s local neighborhood. GraphSAGE utilizes three aggregator functions; Mean, LSTM and pooling aggregators.

GL-Coarsener represents the coefficient matrix as a graph, enabling the implementation of state-of-the-art embedding algorithms such as those mentioned in this section. A precise graph embedding plays an essential role in an effective coarsening.

Learning graph latent features has always been an interesting topic in network analysis field. In this paper, we use node2vec [19], a graph representation learning algorithm that learns node features in a graph using machine learning techniques.

The goal of graph representation learning is to map each node of the network \( G(V, E) \) to a \( d \)-dimensional vector in the embedding space \( Z \) in a way that similar nodes in the graph are close to each other in the \( d \)-dimensional embedding space. This allows us to encode network information and generate node representation. The Embedding Module in Fig. 2 illustrates a two-dimensional representation of a graph.

We can use different metrics to measure the similarity of the nodes in the embedding space; here we are using cosine similarity (dot product) [19]:

\[
\text{similarity}(u,v) \approx z_v^T z_u
\]  

(5)

For measuring the similarity of the nodes in the original graph we will use random walk approach. We will explore the graph by applying \( \gamma \) random walks of length \( t \) on each node and define the similarity of nodes \( u \) and \( v \) as the probability that \( u \) and \( v \) co-occur on a random walk over the network.

Each random walk generates a set of neighbors for each node. For example, for node \( u \) random walk approach generates \( N(u) \).

To generate the embedding vectors, we can view this as an optimization problem with the goal of maximizing the similarity of the neighboring nodes obtained from random walks [19]:

\[
\max_{u \in V} \prod_{v \in N(u)} P(N(u) | z_u)
\]  

(6)

To obtain the embedding space similarity, Eq. 6 calculates the product of all node similarities. Multiplying the probabilities, will cause the result to vanish quickly. To address this phenomenon, we take the log of Eq. 6:

\[
\max \left( \log \prod_{v \in N(u)} P(N(u) | z_u) \right)
= \max \sum_{u \in V} \log P(N(u) | z_u)
\]  

(7)

The optimization problem could be redefined as minimizing the loss function:

\[
\mathcal{L} = \sum_{u \in V} \sum_{v \in N(u)} -\log P(v | z_u)
\]  

(8)

where \( P(v | z_u) \) is the probability of reaching node \( v \) in the random walks given that we started the walk from node \( u \).

By minimizing the above equation, we get an embedding space that nodes \( u \) and \( v \) are closer if they are neighbors in the random walks obtained from the graph.

To parameterize \( P(v | z_u) \), we will use softmax [23]:

\[
P(v | z_u) = \frac{\exp(z_v^T z_u)}{\sum_{n \in V} \exp(z_n^T z_u)}
\]  

(9)
Softmax ensures that the output is between 0 and 1. The equation above is simply used so that node $v$ be most similar to node $u$ out of all nodes $n$.

Putting it all together, we have:

$$L = \sum_{u \in V} \sum_{v \in N(u)} -\log \frac{\exp(z_u^T z_v)}{\sum_{n \in V} \exp(z_u^T z_n)}$$  \hspace{1cm}(10)

Optimizing the random walks basically means finding the embeddings $z_u$ that minimizes $L$.

The problem with the above equation is that nested sum over all nodes in the graph is computationally very expensive, it gives a computational complexity of $O(|V|^2)$. To address this issue, the sum over all nodes in the softmax equation could be approximated as [19]:

$$\log \frac{\exp(z_u^T z_v)}{\sum_{n \in V} \exp(z_u^T z_n)} \approx \log \sigma(z_u^T z_v) - \sum_{i=1}^{k} \log \sigma(z_u^T z_{n_i})$$  \hspace{1cm}(11)

In the above equation, $\sigma$ is the sigmoid function and $n_i$ is selected randomly from all nodes in the graph. This technique is called negative sampling [24]. Instead of normalizing the cosine similarity with respect to all nodes, we just normalize against $k$ random negative samples $n_i$. Higher $k$ gives a more robust estimates.

Now that the general optimization based algorithm was explained, we will discuss two different methods that could be used for generating random walks; DeepWalk and node2vec.

**DeepWalk** is the simplest random walk approach. For generating the random walks, it will start from a given node and selects the next node randomly based on uniform distribution, generating an unbiased random walk.

The next method is **node2vec**. The idea of node2vec is to generate a biased random walk that can trade off between local (micro) and global (macro) views of the graph. It is done by biased 2nd-order random walks that explore network neighborhoods.

**node2vec** introduces two tunable parameters: Return parameter $p$ and In-Out parameter $q$. As show in Fig.3, these two parameters allow us to move between the two extreme Breadth-First Search (BFS) and Depth-First Search (DFS) approaches.
As shown in Fig. 4 for a BFS-like walk we need to provide a low value of \( p \) and for a DFS-like walk we need a low value of \( q \).

### 3.2.2 K-Means

The goal of clustering is to divide the data points into clusters such that the elements assigned to a particular cluster are similar in some predefined sense. Clustering algorithms are divided into two major categories, global and local clustering. In global clustering, every data point is assigned to a cluster in each iteration; whereas in a local approach, the algorithm uses crawlers to explore the data points and assign only a subset (usually one) of nodes to a cluster [25].

K-means is a global clustering method originally proposed in 1967 [26]. The main idea is to group points into clusters with the nearest centroids. Algorithms such as K-Means++ [27] and Mini-Batch K-Means [28] drastically improve K-mean’s performance when large-scale data sets are handled. Currently, K-means and methods based on it are widely used for cluster analysis in machine learning applications.

The coarsening scheme introduced in this work is an aggregation based method which uses the preliminary prolongation matrix \( \hat{P} \) (Eq. 3) as the transfer operator. node2vec algorithm is used for the embedding module; these embeddings are then utilized by K-Means in the clustering module to aggregate the nodes.

K-Means is a clustering algorithm that tries to divide \( N \) samples into \( K \) disjoint clusters \( C \). K-Means initializes \( K \) randomly selected centroids in the sample space and each node is assigned to the closest centroid. The idea is to iteratively update centroid positions so that sum-of-squares of the distances from the corresponding centroids is minimized:

\[
\arg\min_{\mathbf{C}} \sum_{i=1}^{k} \sum_{x \in C_i} ||x - \mu_i||^2 \tag{12}
\]

K-Means++ introduces an improvement on initialization algorithm and selecting the initial positions of the centroids. Selecting centroids intelligently increases the speed of K-Means clustering algorithm [27].

K-Means clustering algorithm does not scale well to large number of samples. Since the graphs that we are working with usually contain more than 10k number of nodes, we are using a customized version of K-Means called Mini-Batch K-Means [28].

Mini-Batch K-Means applies the same K-Means algorithm but it doesn’t run the algorithm on all of the samples at the same instance. It divides the original samples to multiple batches and then runs the algorithm on each batch of samples.

#### Algorithm 2 Mini-Batch K-Means [28]

**Input:** \( k \), mini-batch size \( b \), iterations \( t \), data set \( X \)

**Output:** Clusters

1. \( v \leftarrow 0 \)
2. for \( i = 1 \) to \( t \) do
3. \( M \leftarrow b \) samples picked randomly
4. for \( x \in M \) do
5. \( d[x] \leftarrow f(C, x) \) \( \rightarrow \) Cache nearest center to \( x \)
6. for \( x \in M \) do
7. \( c \leftarrow d[x] \) \( \rightarrow \) Get cached center for this \( x \)
8. \( v[c] \leftarrow v[c] + 1 \) \( \rightarrow \) Update per-center counts
9. \( \eta \leftarrow \frac{1}{v[c]} \) \( \rightarrow \) Get per-center learning rate
10. \( c \leftarrow (1 - \eta)c + \eta x \) \( \rightarrow \) Take gradient step

#### 4 PROPOSED METHOD

In this paper, we propose GL-Coarsener framework. GL-Coarsener aims to cluster fine grid based on nodes’ neighbors in the underlying graph. These clusters will then be aggregated to form the coarse grid. Then, the residual equation (Eq. 4) will be solved on the coarse grid, and finally, the correction in the coarse grid will be transferred to the fine grid and added to the approximate solution. In the following sections we explain the process step by step.

#### 4.1 Pre-Processing

In the AMG context, we are usually dealing with very large sparse matrices. To facilitate working with extensive data and use memory more efficiently, we convert the data to CSR (Compressed Sparse Row) format. In CSR format, only the non-zero elements of the sparse matrix will be stored, and there will be enough information to restore the original matrix elements when needed.

We need to convert matrix \( A \) in Eq. 4 to a graph. Matrix \( A \) corresponds to the original grid’s underlying graph, with each element in \( A \) indicating the weight of edges of the graph. For example, \( A_{ij} \) represents the weight of the edge that connects node \( i \) to node \( j \).
4.2 Algorithm

The first step of our proposed AMG algorithm is pre-smoothing. In this step, we will try to reduce high-frequency errors that exist in the approximate solution. To do this, we will use numerical iterative solvers (e.g., Jacobi, Gauss-Seidel). A few iterations as low as 1-5 suffice to reduce high-frequency errors in most cases:

\[ Av = f \]
\[ Jacobi: \ v^{(k+1)} = D^{-1}(f - (L + U)v^{(k)}) \] (13)

where \( A = L + D + U \) and \( L, D \) and \( U \) are lower triangular, main diagonal and upper triangular sub-matrices of \( A \), respectively.

After performing a few iterations, the iterative solver’s convergence rate drops drastically to the point that there is no noticeable improvement in the solution. This significant drop in convergence rate indicates that the iterative solver has reached its limit on the current grid.

That indicates that we need to find a coarser level representation of the system. The system’s low-frequency errors will become high frequency at the coarse level, therefore the convergence rate is recovered.

To do this, we will apply graph representation techniques to generate the embedding space of the graph. As said earlier, we will use node2vec algorithm. As shown in the Embedding Module of Fig. 2, node2vec maps similarities of the graph to the embedding space so that the nodes which are neighbors in the graph, would be closer to each other in the embedding space. As explained in section 3.2.1, node2vec algorithm generates vectors of size \( d \) for each node in order to represent the graph in a \( d \)-dimensional space.

Afterward, we will feed the newly obtained embedding space to the K-Means clustering algorithm. As shown in the Clustering Module of Fig.2, K-means clustering algorithm receives the embedding vectors and the number of clusters as input and will assign similar nodes into the same cluster. In this work, we will use \( \frac{d}{2} \) as the number of clusters, meaning that there will be approximately five nodes in each cluster of nodes.

For the example shown in Fig.5 K-Means clustering algorithm has successfully assigned neighboring nodes of the original grid in to the same clusters.

If our graph size is large (more than 10k nodes), the K-Means clustering algorithm might take too long to finish. In this case, as explained above modified version of the algorithm called Mini-Batch K-Means is used. As explained in section 3.2.2, Mini-Batch K-Means accurately approximates the K-Means clustering algorithm much faster.

After generating the clusters, we will construct the coarse level coefficient matrix. This step differentiates aggregation-based AMG methods. To do that, we will use Standard Aggregation method [11].

Standard Aggregation method proposes a simple approach for constructing the prolongation operator, which will be used to construct the coarse level equation system. The prolongation operator could be either rough or smooth. A rough prolongation operator could be constructed as shown in Eq. 3. In small problems, rough aggregation yields a faster convergence.

Using iterative methods like Jacobi, damped Jacobi, Gauss-Seidel and SOR, we could smooth the rough prolongation operator and get a smoother operator:

\[ P_f = (I - D^{-1}A)\hat{P} \]
\[ P_{\omega J} = (I - \omega D^{-1}A)\hat{P} \]
\[ P_{GS} = (I - (D - L)^{-1}A)\hat{P} \]
\[ P_{SOR} = (I - \omega(D - L)^{-1}A)\hat{P} \] (14)

\( D \) is the main diagonal of coefficient matrix \( A \), \( L \) is the strictly lower triangular part of \( A \), and \( \omega \) is the damping or relaxation parameter.

Once the prolongation operator is constructed, we need to find the residual of system using the approximate solution calculated in pre-smoothing step of the AMG. This could be achieved using Eq. 4. The residual equation is then transferred to the coarse level:

\[ A_c = P^T AP \]
\[ r_c = P^T r \] (15)

This gives the coarse grid equation as:

\[ A_c e_c = r_c \] (16)

Now, we need to solve Eq. 16 for \( e_c \). \( e_c \) on the coarse level corresponds to the correction we need to make on the fine level. Unlike the residual equation in fine level, the system in coarse level features has relatively high-frequency errors. This equation could be solved recursively using the same AMG principles.

After solving the residual equation on the coarse level, using the prolongation operator, we need to transfer back
the correction calculated on the coarse grid and add the correction to the approximate solution found in pre-smoothing step.

\[ e = Pe_c \]
\[ u = v + e \]  

(17)

Algorithm 3 One iter. of our proposed AMG method

1: function V-CYCLE\((A_f, f_f, v_f)\)
2: \( n \leftarrow \text{length of } f_f \)
3: \( v_f \leftarrow \text{smoothing}(A_f, f_f, v_f) \) \hspace{1em} \triangleright \text{Pre-Smoothing}
4: \( r_f \leftarrow f_f \cdot A_f v_f \)
5: \( \text{embedding} \leftarrow \text{node2vec}(A_f) \)
6: \( \text{clusters} \leftarrow \text{MiniBatchKMeans(embedding, } \left\lceil \frac{n}{4} \right\rceil \) \)
7: initialize \( P \) to be an \( n \) by \( \left\lceil \frac{n}{4} \right\rceil \) matrix
8: for \( i \leftarrow 0 \) to \( n \) do
9: \hspace{1em} for \( f \leftarrow 0 \) to \( \left\lceil \frac{n}{4} \right\rceil \) do
10: \hspace{2em} if \( i \in \text{clusters}[j] \) then
11: \hspace{3em} \( P_{ij} \leftarrow 1 \)
12: \hspace{1em} else
13: \hspace{2em} \( P_{ij} \leftarrow 0 \)
14: \end{algorithm}
15: \( R \leftarrow P^T \)
16: \( A_c \leftarrow \text{RAP} \)
17: \( r_c \leftarrow R r_f \)
18: if Coarsest Grid Achieved then
19: \hspace{1em} Solve \( A_c e_c = r_c \) for \( e_c \)
20: else
21: \hspace{1em} \( r_c \leftarrow \text{V-CYCLE}(A_c, r_c, e_c) \)
22: \hspace{1em} \( e_f \leftarrow P r_c \)
23: \hspace{1em} return \( v_f + e_f \)

4.3 Code

The code for our proposed method is available in two forms. GL-Coarsener \[3\] could be used as a stand-alone module to reduce the size of a large graph. A modular code \[4\] for AMG is also available that could be used to solve large systems of equations.

5 NUMERICAL EXPERIMENTS

This section compares the performance of our proposed AMG method with different graph-based and aggregation-based AMG methods. These methods include Beck’s graph-based method and Vanek’s standard aggregation-based method.

In this section we report implementation of the methods described so far to solve linear systems arising from discretization of the Poisson’s equation:

\[ \Delta \varphi = f \]  

(18)

where \( \Delta \) is the Poisson’s operator, \( \varphi \) and \( f \) are real or complex valued functions.

The discretization is handled by Rayan [29] using Finite Volume Method (FVM) and is treated as the input to the current work. The Poisson’s problem is a typical problem occurring in modeling of many physical systems including heat transfer, fluid flow and electrostatics. It is common to solve this problem on grids ranging from a few hundred degrees of freedom (unknowns) to millions and occasionally a few billions (for complex research or industrial problems).

5.1 Method Setup

In what follows the details of settings used in the numerical experiments are described.

5.1.1 AMG V-Cycle

The method proposed herein is applicable to all of multi-grid strategies (for example, V, W and F cycles). For demonstration, we will use it in conjunction with V-cycle. Properly setting up the V-Cycle plays a crucial role in its convergence rate. For the pre-smoothing step of the V-Cycle, we use two iterations of Jacobi smoothing. The reason for choosing Jacobi over other iterative solvers like Gauss-Seidel is its natural high potential for parallel application. Our proposed method is also naturally highly parallel and therefore selecting a matching smoother makes the overall set up consistent for massively parallel applications. After each iteration of V-Cycle, we apply seven more Jacobi post-iterations; we found it very effective to damp the remaining high-frequency errors.

Since solving large systems directly is computationally very expensive, we will recursively construct coarser grids to the point that we reach a system with 20 unknowns or less. We then solve the system directly.

For a given system of equations, we need to solve the system over multiple iterations of V-Cycle. Evidently, the construction of the prolongation operators happens just on the first iteration of V-cycle and this prolongation operators are reused for the rest of iterations.

5.1.2 node2vec

The purpose of node2vec embedding module is to map the underlying graph of the system’s adjacency matrix to a \( d \)-dimensional embedding space. \( d \) is a hyper-parameter of node2vec that needs to be chosen with care. If we choose a too low value for \( d \), the embedding space is not large enough to capture all the latent features of the graph and if we choose an excessive number of dimensions for our embedding space, the model takes too long to train and it adversely affects the performance of the method. By running multiple experiments and comparing the results to the standard aggregation method, we found an embedding dimension of 128 to be sufficient to capture latent features of systems with up to 1.5 millions unknowns.

To explore the graph, node2vec needs two hyper-parameters \( p \) and \( q \). In AMG aggregation-based methods, we aim to aggregate neighboring nodes in the same cluster, therefore a local view of the graph is more desirable than a global view. As described in section 3.2.1, a low value \( p \) gives us a BFS-like search of the graph resulting in a local view. Here we choose return parameter \( p \) to be

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\[3\] Available at \url{https://github.com/rezanmz/GL-Coarsener}

\[4\] Available at \url{https://github.com/rezanmz/AMG}
0.1 and in-out parameter $q$ to be 1. However, numerical experiments indicated that the GL-Coarsener algorithm is not much sensitive to values of $p$ and $q$. We also choose to run $2 \times \text{AverageDegree}$ walks of length 10 to make sure that we capture all the neighbors.

### 5.1.3 Mini-Batch K-Means

To generate the clusters of neighboring nodes in the embedding space, we use Mini-Batch K-Means. If we choose the number of clusters to be very low, we will lose too much information when we move between fine and coarse level; and if the number of clusters is very high, in large systems we will have a very long hierarchy of coarser levels; therefore, the runtime increases. By numerical experiments, we found that if we approximately cluster every 5 nodes of the original fine graph into a cluster, we get a good convergence rate; therefore, we choose the number of clusters to be $\frac{n}{5}$. To run the clustering algorithm faster, we choose a batch size of $\frac{n}{15}$.

### 5.2 Evaluation

We evaluate the performance of the AMG methods with V-Cycles of dynamic depth, meaning that we recursively construct coarser grids to the point we reach a linear system with 20 unknowns or less. The system is then solved directly, and the coarse correction is interpolated back on the respective fine grid. After each iteration, we compute the infinity norm of the residual:

$$\|r\|_{\infty} := \max(|r_1|, \ldots, |r_n|)$$

### 5.2.1 Stopping Criteria

Since AMG is an iterative method computing successive approximations to the solution, we should use stopping criteria to determine when to stop iterating. In these experiments, we use:

$$\|r\|_{\infty} < 10^{-4}$$

as the stopping criterion for the iterative method.

### 5.3 Results

![Multigrid V-Cycle Comparison](image)

Fig. 6. A comparison of different AMG methods with stopping criteria of $\|r\|_{\infty} < 10^{-4}$. For systems larger than 128k unknowns, performances of Beck and Standard Aggregation methods were projected using extrapolation techniques. Graph-based methods (like Beck) generally have lower convergence rate than aggregation-based methods (like our methods and Vaněk’s standard aggregation).

| System Size | Beck | Vaněk | Proposed Method |
|-------------|------|-------|-----------------|
| 1k          | 186  | 49    | 64              |
| 2k          | 366  | 80    | 95              |
| 4k          | 691  | 110   | 157             |
| 8k          | 1419 | 158   | 260             |
| 16k         | 2743 | 269   | 412             |
| 32k         | 5627 | 356   | 605             |
| 64k         | 10709| 540   | 987             |

Table 1. A comparison between multi-grid methods. The data points indicate iterations needed to solve different systems with stopping criteria of $\|r\|_{\infty} < 10^{-4}$.

As shown in Fig. 6 as the size of the system increases, the number of iterations needed for our method increases linearly, closely following Vaněk’s standard aggregation-based method and much better than a typical graph based method. Table 1 shows the data used to generate Fig. 6.

### 6 CONCLUSION

In this paper we propose an aggregation-based AMG method. In our proposed method, we use powerful machine-learning and deep-learning techniques to learn the mappings between coarse and fine levels of AMG’s V-Cycle. First, we map the system’s underlying graph to a $d$-dimensional embedding space, then we use Mini-Batch K-Means clustering method to find clusters of neighboring nodes in the system. Using the method provided in Vaněk’s standard aggregation, these clusters are then used to construct the prolongation operator that map the fine level to the coarse level. It has been demonstrated that the GL-Coarsener framework while relying on machine learn-

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5In a graph, average degree is simply the average number of in/out edges per node: $\text{AverageDegree} = \frac{|\text{Edges}|}{|\text{Nodes}|}$. 

ing techniques performs well compared to other existing AMG methods. Another advantage of the method is its naturally parallel characteristic.

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