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Harnessing High-Performance Computing for Carbon Capture and Storage: A Strategic Pathway to Climate Change Mitigation

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ABSTRACT

Introduction: The accelerating pace of climate change, driven primarily by rising greenhouse gas emissions, presents a critical challenge to sustainable natural resource management. Carbon Capture and Storage (CCS) is increasingly recognized as a viable mitigation strategy to reduce atmospheric CO_2 levels and support global carbon neutrality goals. **Methods:** This study explores the integration of Machine Learning (ML)—specifically Graph Convolutional Networks (GCNs)—and High-Performance Computing (HPC) to optimize CCS processes. GCNs are employed to analyze and model complex datasets for CO_2 transport, identifying optimal routes based on criteria such as distance, cost, and efficiency. Simultaneously, HPC infrastructure, including GPU acceleration, is leveraged to enhance computational speed and processing capabilities. **Results:** The combined implementation of GCNs and HPC significantly reduces computational time—by approximately 65% compared to GCNs without HPC support. This acceleration enables real-time route optimization and model recalibration based on dynamic environmental and logistical inputs, improving the operational efficiency of CO_2 capture, transport, and storage. **Conclusions:** The integration of high-performance computing with advanced ML techniques offers a transformative approach to improving CCS systems. By enabling rapid, data-driven decision-making, this strategy not only enhances the precision and efficiency of CCS but also strengthens broader efforts toward climate change mitigation and sustainable environmental management.

Keywords: Carbon Capture and Storage, Climate Change, Computational Modeling, Green Technology, High-Performance Computing, Machine Learning, Sustainability, Transportation

1. INTRODUCTION

Rapid climate and environmental changes present significant challenges for global natural resource management, primarily driven by increased greenhouse gas emissions, particularly carbon dioxide (CO_2). These changes have severely impacted ecosystems, economies, and human quality of life (Intergovernmental Panel on Climate Change [IPCC], 2021). Researchers have recently developed technologies to reduce CO_2 emissions, as they significantly contribute to global warming (Friedlingstein, et al., 2022). One key approach is Carbon Capture and Storage (CCS) technology, which is essential for lowering

CO_2 levels in the atmosphere. The primary goal of CCS is to safely and permanently store CO_2 underground, making it a crucial strategy for achieving the ambitious goals of Carbon Neutrality and Net Zero Emissions (Bui, et al., 2018). However, the large-scale CCS implementation challenges related to efficiency and cost, especially concerning the transportation of CO_2 from emission sources to storage sites. Designing efficient transportation routes is crucial for economic feasibility and widespread CCS adoption. Integrating Machine Learning (ML) and High-Performance Computing (HPC) shows great promise in revolutionizing CCS system design and operation (Wim, et al., 2013), potentially overcoming these challenges and enhancing the technology's effectiveness in combating climate change.

ML can be applied to analyze various factors related to CO_2 transportation and geoinformatics, such as distance, terrain, traffic patterns, and existing infrastructure. Given the large and complex nature of these datasets, ML techniques can be employed to optimize route selection for CO_2 transport. This optimization may involve identifying the shortest, the fastest, or the most cost-effective path from the source to the sink. Meanwhile, HPC is essential for supporting ML operations, as it can process large amounts of data quickly and accurately (Ettifouri, et al., 2024). HPC resources, including Graphics Processing Units (GPUs), enable rapid computation and modeling of complex scenarios. This capability is particularly crucial for analyzing and designing CO_2 transportation routes from multiple emission sources to storage sites (sinks) across a country or region (Yan, et al., 2021).

The integration of ML and HPC in advancing and refining CCS systems not only improves the effectiveness of reducing atmospheric CO_2 but also reduces expenses and enhances the practicality of widespread CCS implementation (Wen, et al., 2021). Thus, the objective of this research is to demonstrate the application of ML in conjunction with HPC to identify the shortest path from CO_2 emission sources to sinks. This research explains how HPC can reduce processing time, making CO_2 transportation in real-world applications more efficient.

2. MATERIALS AND METHODS

This section provides the details of the datasets and optimization algorithms, such as Dijkstra's algorithm and Graph Convolutional Networks (GCN), utilized to determine the most efficient routes for CO_2 transportation in Thailand.

2.1. Datasets

The datasets incorporate 1,956 CO_2 emission sources dispersed across Thailand and two potential sinks for CCS projects, specifically the Lampang Basin in northern Thailand and the basin in the Gulf of Thailand. Furthermore, this research necessitates the use of HPC systems to determine the optimal route among all possible paths between emission sources and sinks across the country.

2.2. Dijkstra's Algorithm

Dijkstra's algorithm is employed to determine the shortest path between nodes in a graph (Noto & Sato, 2000). In this study, the graph consists of CO_2 emission sources represented as nodes, with sinks designated as destination nodes. The edges of the graph illustrate the road network within the country, weighted by distance between each node. The algorithm constructs a tree of shortest paths from the emission sources to the destination sinks. It operates by maintaining a set of unvisited emission sources and calculating tentative distances from a source node to each destination sink. When a shorter path to a particular node is identified, the algorithm updates the corresponding distance. This problem demonstrates an optimal substructure as follows: if CO_2 emission source A (the starting node) is connected to CO_2 emission source B and CO_2 emission source B is linked to a destination sink (the destination node), such that the path from CO_2 emission source A to the destination sink must pass through CO_2 emission source B, then the shortest path from CO_2 emission source A to CO_2 emission source B, together with the shortest path from CO_2 emission source B to the destination sink, constitutes the overall shortest path from CO_2 emission source A to the destination sink. Therefore, the optimal solutions to these subproblems directly inform the overall optimal solution, facilitated by the algorithm's systematic tracking of the shortest possible path to each node.

2.3. Graph Convolutional Networks (GCN)

A GCN is a specific type of Graph Neural Network (GNN) designed to process and analyze graph-structured data. In this context, a graph consists of interconnected nodes and edges, where nodes represent entities and edges denote the relationships or connections between them. Unlike traditional Convolutional Neural Networks (CNNs), which operate on grid-like data such as images, GCNs perform convolutional operations on an adjacency matrix (Suetrong, et al., 2024) or a node feature matrix.

In this work, the nodes represent various sources and sinks, while edges represent the connections between these nodes, determined by road networks in Thailand. This approach is similar to Dijkstra's algorithm, as previously mentioned. The nodes and edges serve as inputs to the GCN model. The model utilizes graph convolutional layers to learn embeddings for the nodes

Table 1. Average training time per epoch of GCN across a total of 20 epochs

Algorithm	Average training time per epoch
GCN without HPC	~ 3.2 hours
GCN with HPC	~ 1.1 hours

Source: Authors, 2024.

Table 2. Average computation time for Dijkstra's algorithm

Algorithm	Average computation time (50 iterations)
Dijkstra's algorithm without HPC	~ 54.49 minutes
Dijkstra's algorithm with HPC	~ 26.74 minutes

Source: Authors, 2024.

based on their connectivity. Ultimately, the model output provides the shortest path between a source and a sink by indicating the next node in the path.

Furthermore, GCNs are a subtype of Deep Learning (DL), which is a branch of ML. GCNs require substantial amounts of data for training and may encounter challenges due to hardware limitations, especially when dealing with very large or complex graphs, such as those with nearly 2,000 nodes in this study. However, HPC resources can adequately support the computational demands associated with training these models.

3. RESULTS AND DISCUSSION

This section analyzes the performance of Dijkstra's algorithm and GCN in identifying the shortest path within a graph consisting of 1,958 nodes (1,956 nodes of sources and 2 nodes of sinks). It compares the training times with and without HPC resources. The local environment used for testing was a 2020 Mac Mini, equipped with an Apple M1 chip featuring an 8-core CPU (4 performance cores and 4 efficiency cores), an 8-core GPU, and 8 GB of memory. In contrast, the HPC environment utilized a 2-core CPU AMD EPYC 7742 @2.25 GHz and a NVIDIA HGX A100 graphics card.

The results indicate that the training time per epoch with HPC is approximately three times faster than without HPC, reducing the duration from around 3 hours to approximately 1 hour. This represents a reduction of about 65%, as shown in Table 1. Furthermore, Table 2 demonstrates that Dijkstra's algorithm runs faster with HPC compared to without, reducing the computation time by approximately 51 %.

4. CONCLUSION

In conclusion, rapid climate changes significantly contribute to global warming. Carbon Capture and Storage (CCS) is a technology aimed at mitigating rising carbon dioxide (CO_2) levels in the atmosphere. It works by capturing CO_2 from emission sources, transporting it to designated sinks, and injecting it underground. This study introduces an application of Machine Learning (ML), particularly Graph Convolutional Networks (GCNs), in conjunction with High-Performance Computing (HPC), which provides substantial computational resources for identifying the shortest path from sources to sinks. The results obtained from both GCN and Dijkstra's algorithm demonstrate that utilizing HPC reduces the training time of the GCN model by approximately 65% and decreases computation time by approximately 51%, respectively. These findings contribute to more efficient management of CO_2 transportation in real-world applications.

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Declaration of Conflicting Interests

The authors declare that they have no competing interests.

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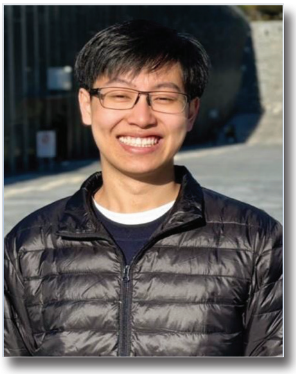

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