PyGim: An Efficient Graph Neural Network Library for Real Processing-In-Memory Architectures

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CentML
VECTOR INSTITUTE

Executive Summary

Problem: The *memory-intensive* kernels of Graph Neural Networks (GNNs) dominate execution time (~91%) and are significantly *bottlenecked by memory bandwidth* in procesor-centric systems (CPUs/GPUs)

Motivation: PIM provide significantly *high memory bandwidth* by enabling computation to be performed close to the application data

PyGim: An *efficient* and *easy-to-use* GNN library for real Processing-In-Memory (PIM) systems

Key Ideas & Benefits:

- Cost Effectiveness: *Heteregenous* GNN kernels are executed in the *best-fit hardware*
- High Performance: (i) Enabling *three levels of parallelism with various strategies* in the PIM side and (ii) *adapting* best-performing parallelization strategy to the graph's *unique characteristics*
- High Programming Ease: (i) Providing a *handy Python API* and (ii) *automatically tuning* the best-fit parallelization strategy without programmer intervention

Key Results: PyGim improves (i) *performance* and *energy efficiency* by **3.7×** and **2.3×** over state-of-the-art schemes, and (ii) *core utilization* on PIM system by **11.6×** over PyTorch on GPUs

github.com/CMU-SAFARI/PyGim

Talk Outline

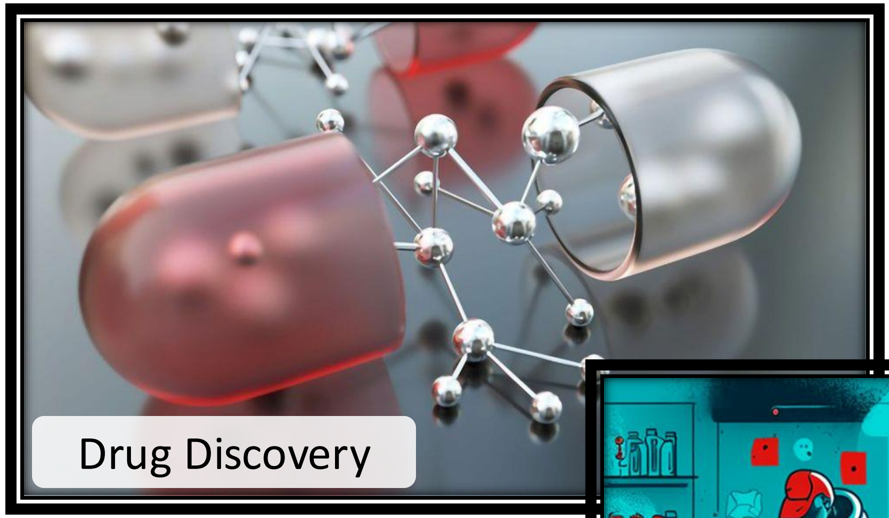
Background & Motivation

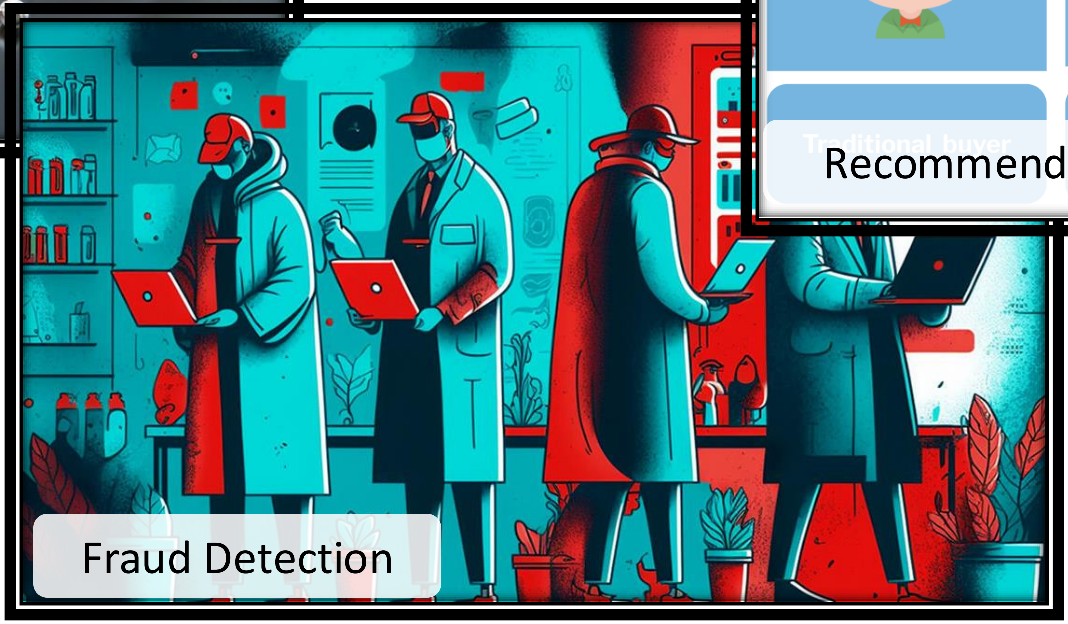
PyGim Design

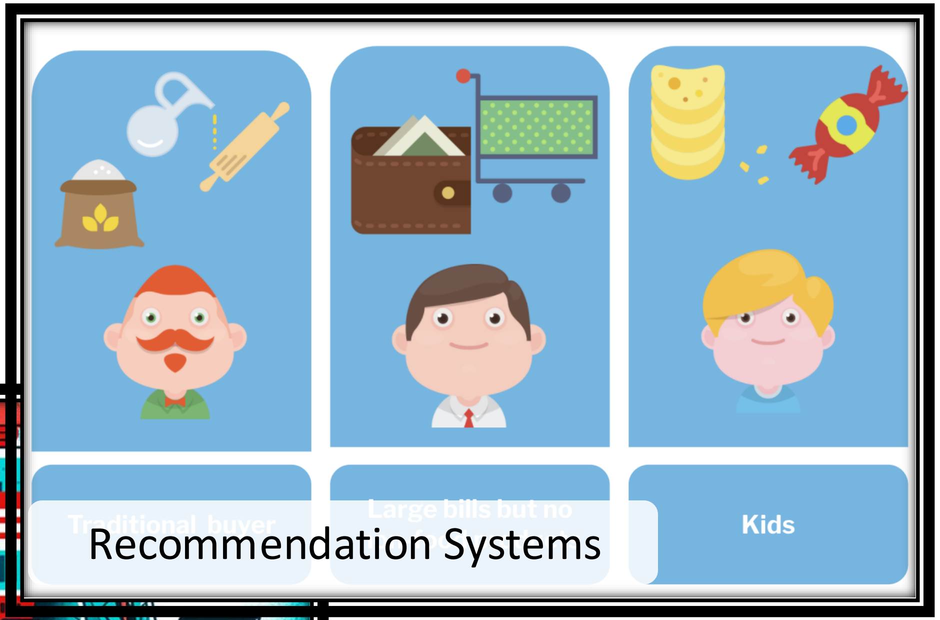
Evaluation

GNNs Are Widely Used in Real-World Applications

- GNNs are state-of-the-art ML models for analyzing graph-structure data
- GNN has a lot of applications:


Drug Discovery

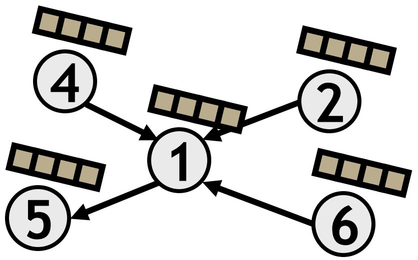

Fraud Detection

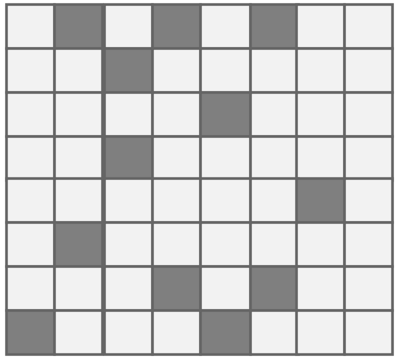


Recommendation Systems

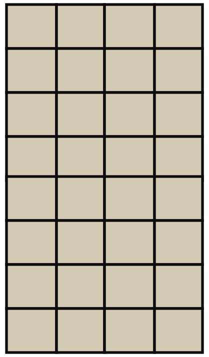
Execution Steps of GNN Layers

- GNNs comprise a few layers (e.g., 3-5 layers)
- Each GNN layer has ***two*** execution steps:





Adjacency (Sparse) Matrix



Input Feature

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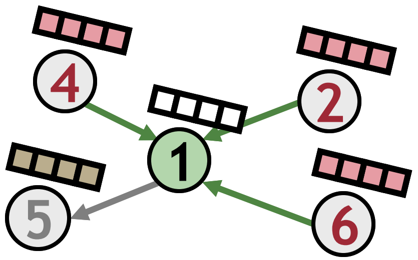

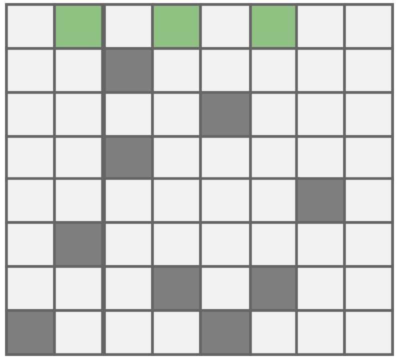

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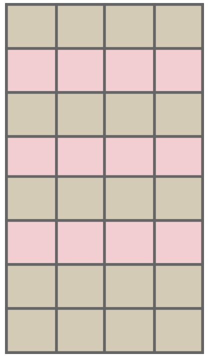

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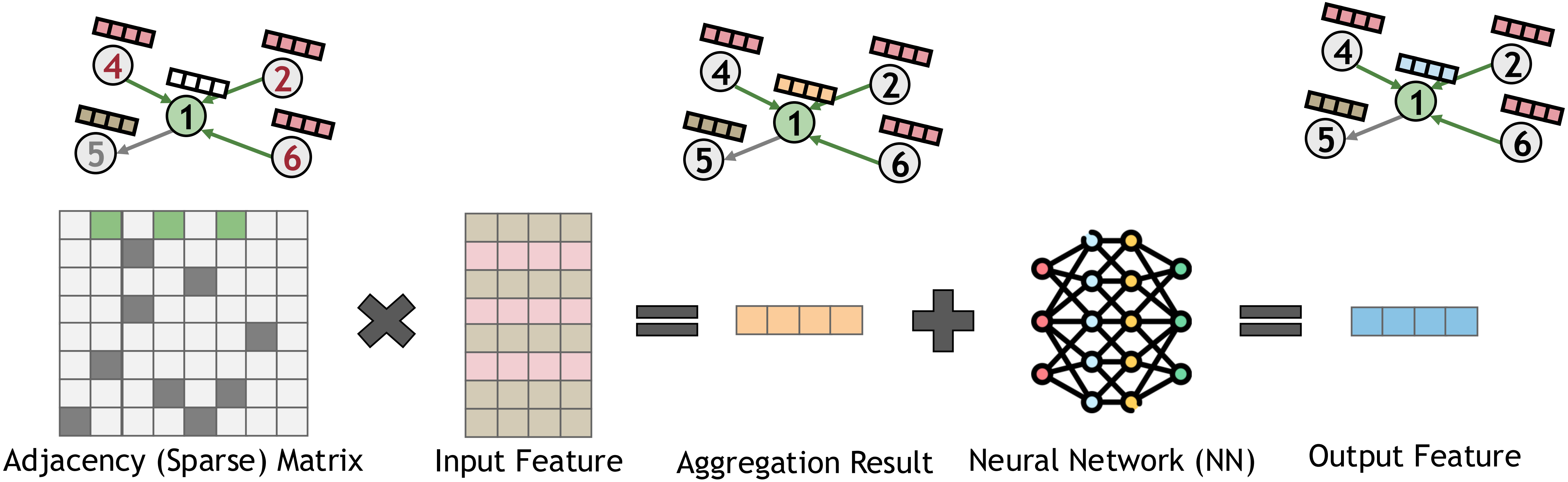

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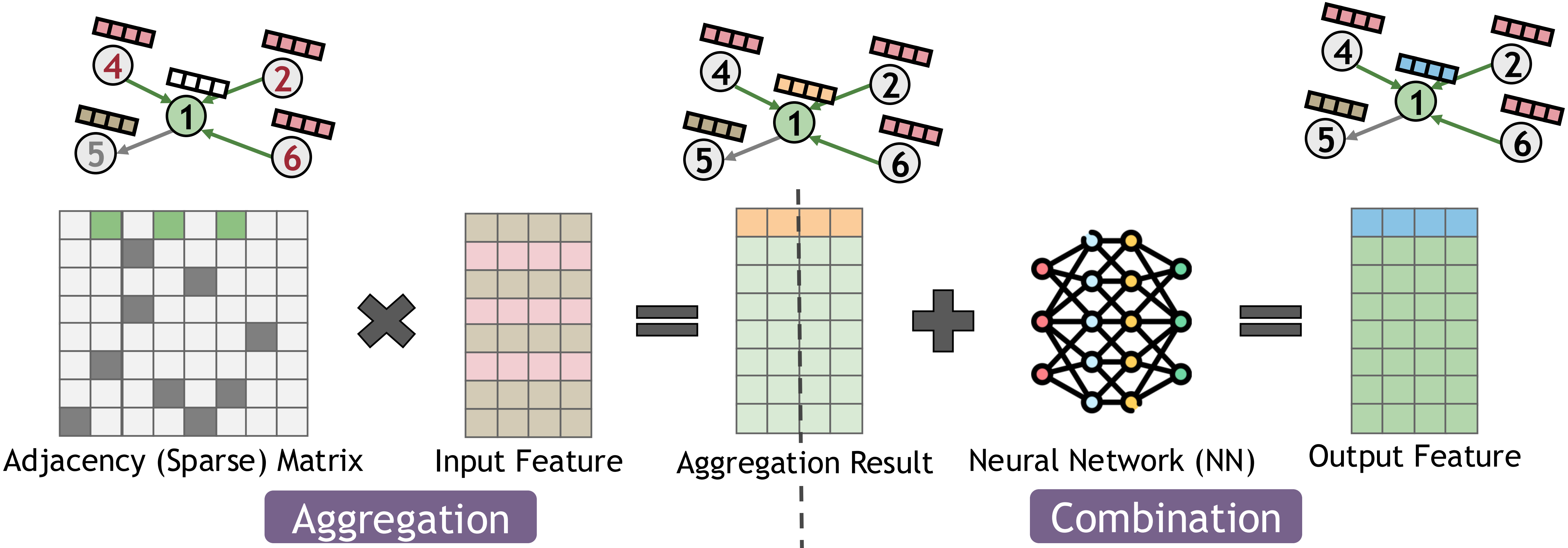
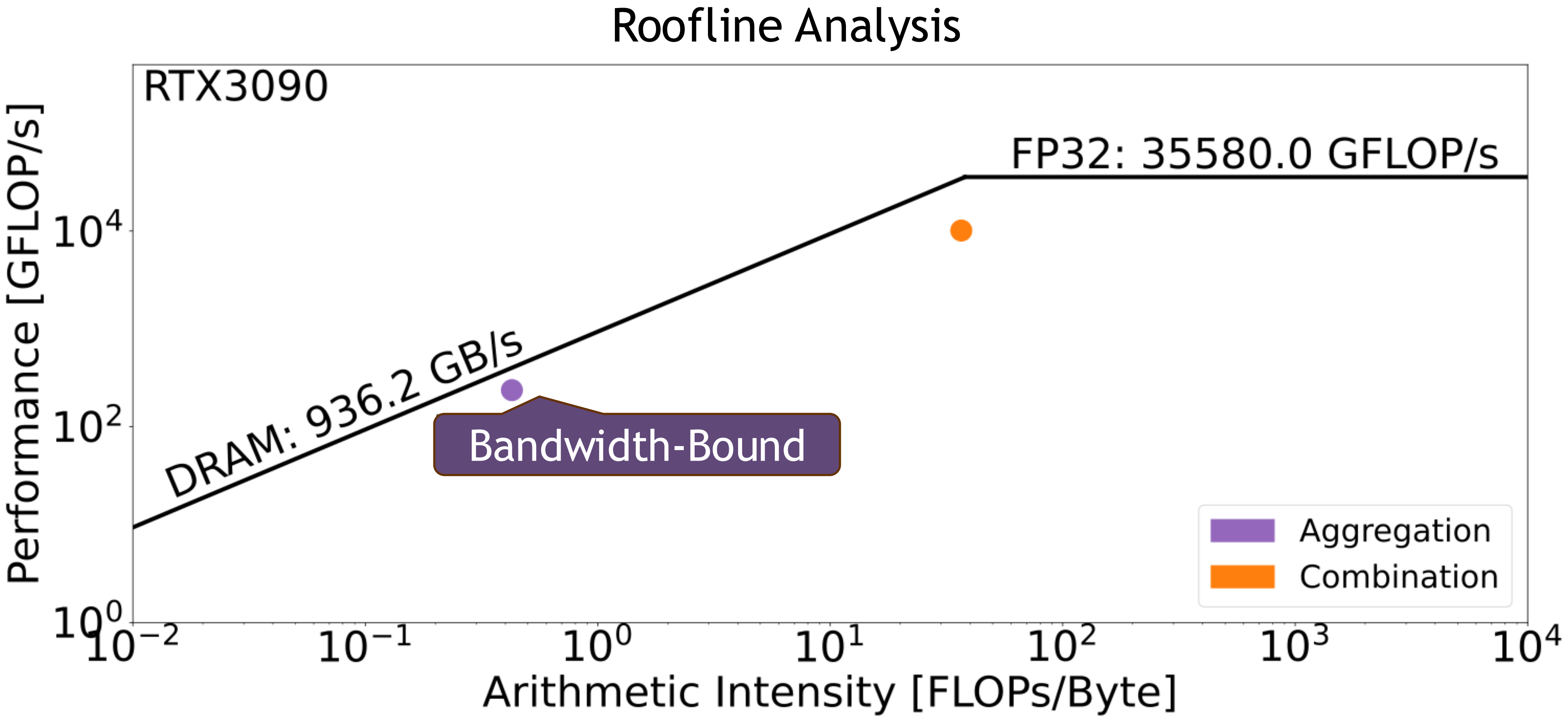


Aggregate neighbor's feature, corresponds to Sparse Matrix Matrix Multiplication (***SpMM***)

Combine features by NN. Typically comprises compute-intensive kernels (e.g., GEMMs)

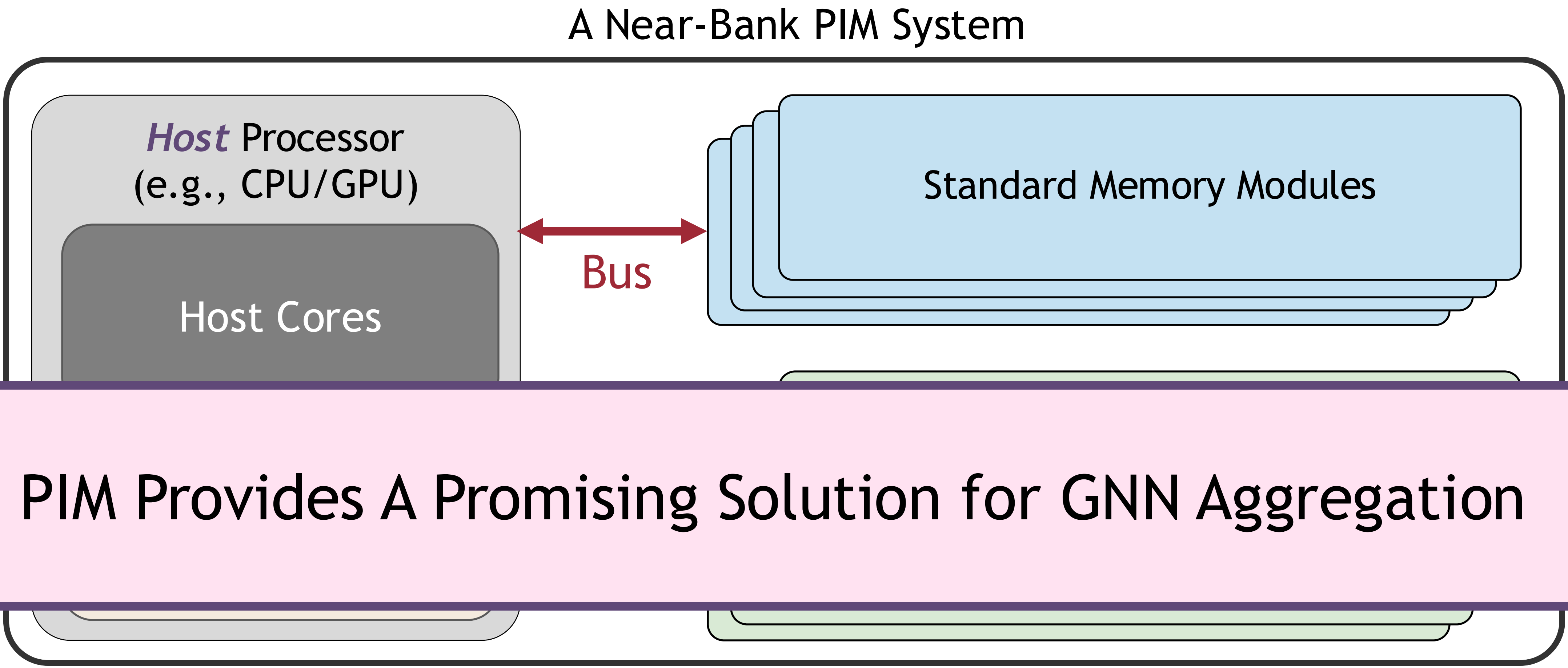
GNN Aggregation Is Memory-Bandwidth-Bound In GPUs

Using a RTX 3090 GPU with ~900 GB/s bandwidth, we find that GNN Aggregation
- takes ***~91%*** of the inference time
- achieves ***less than 2%*** core utilization



PIM Alleviates The Data Movement Bottleneck

- Near-bank PIM: each PIM core is tightly coupled with one (or a few) DRAM banks
- Near-bank PIM cores have significantly higher memory bandwidth than Host cores



PIM Provides A Promising Solution for GNN Aggregation

Talk Outline

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PyGim Design

Evaluation

PyGim Overview

- An efficient and easy-to-use GNN library for real PIM systems
- PyGim incorporates 4 key components:

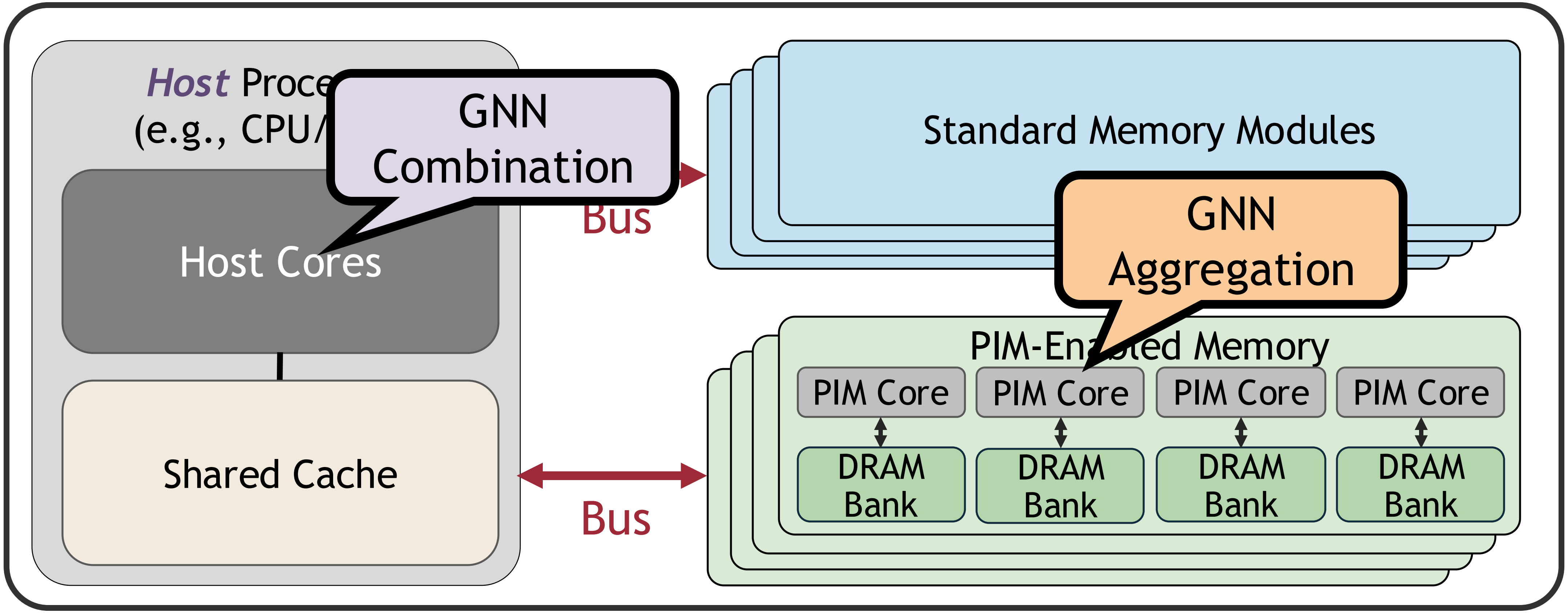
Cooperative Acceleration (CoA)	Run *heterogeneous* kernels in the best-fit hardware
Parallelism Fusion (PaF)	Strives a balance between *computation* and *data transfer*
Lightweight Tuning	*Automatically* tunes the *best-performing* PaF *strategy*
Handy Programming Interface	Integrates a *handy* Python (PyTorch) API

1. Cooperative Acceleration (CoA)

Heterogeneous kernels are running in the best-fit underlying hardware

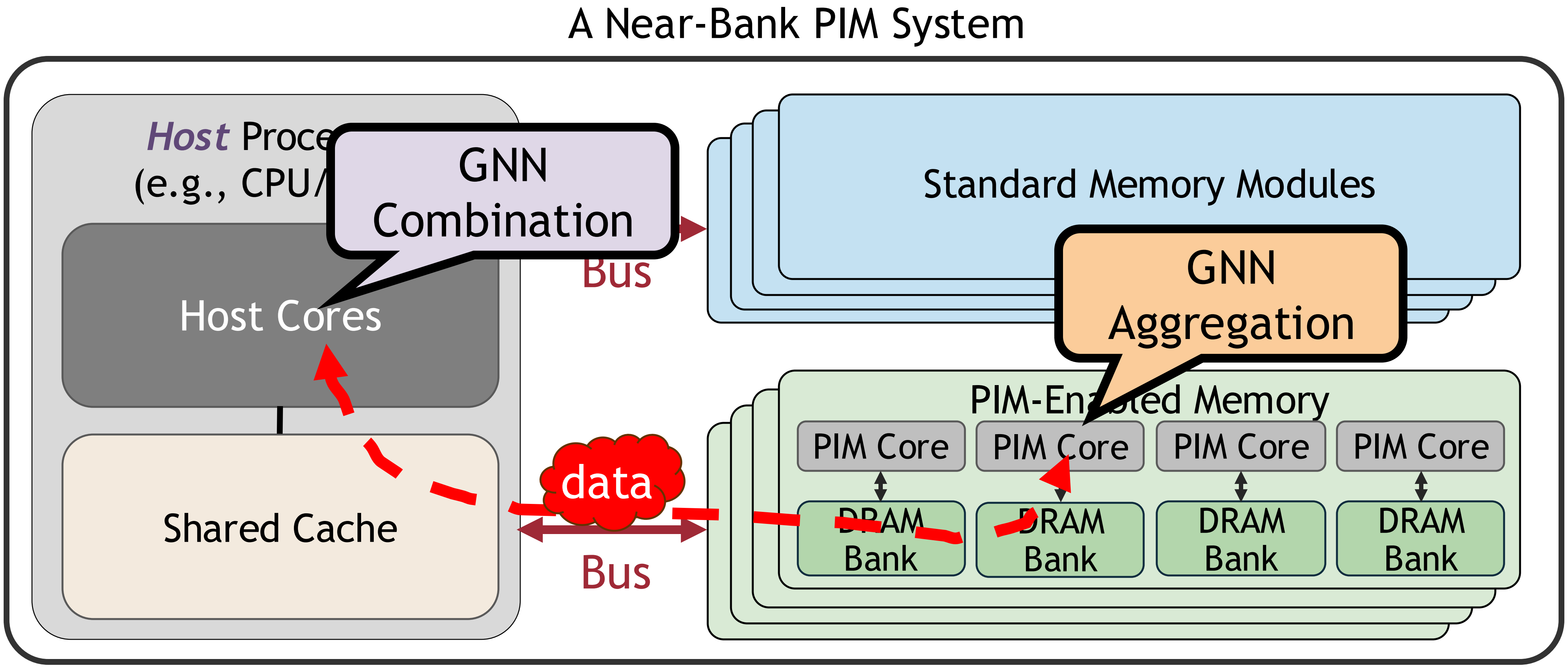
- Combination runs on Host cores
- Aggregation runs on PIM cores

A Near-Bank PIM System



Challenge 1: Expensive Data Transfer Costs

- Alleviate the overheads of passing the output data of the one step as input data to the next step



PyGim Overview

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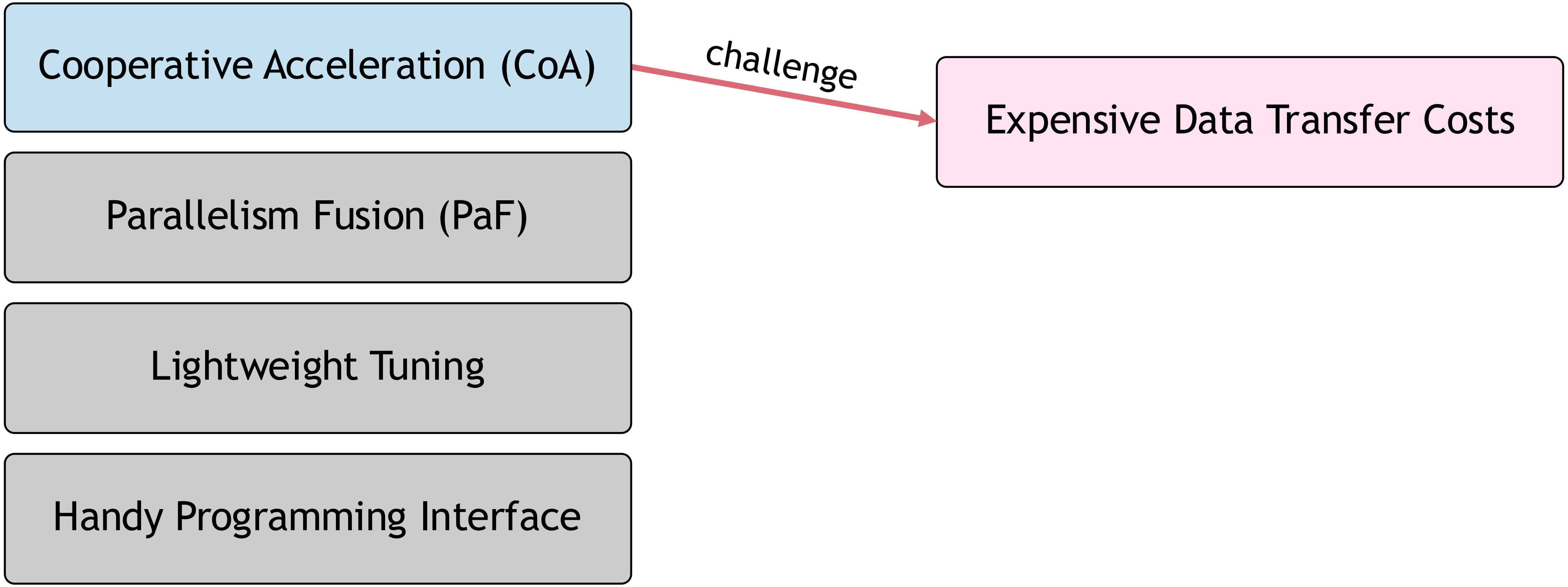

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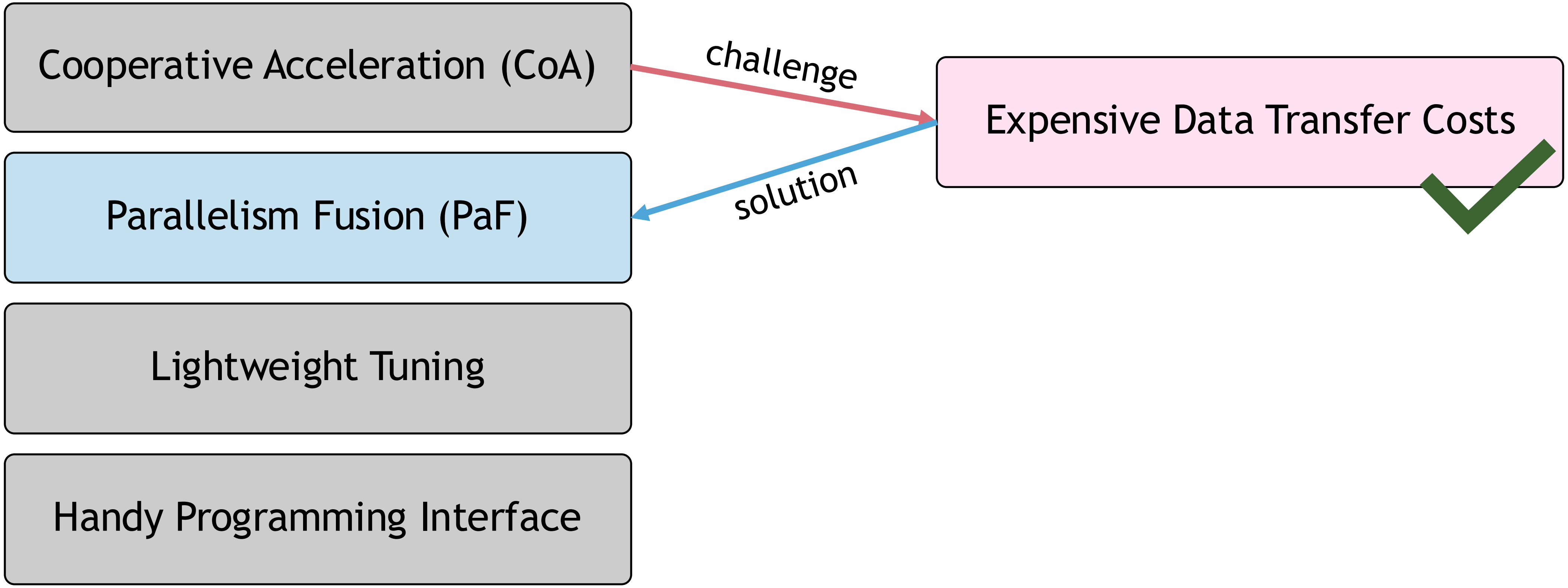
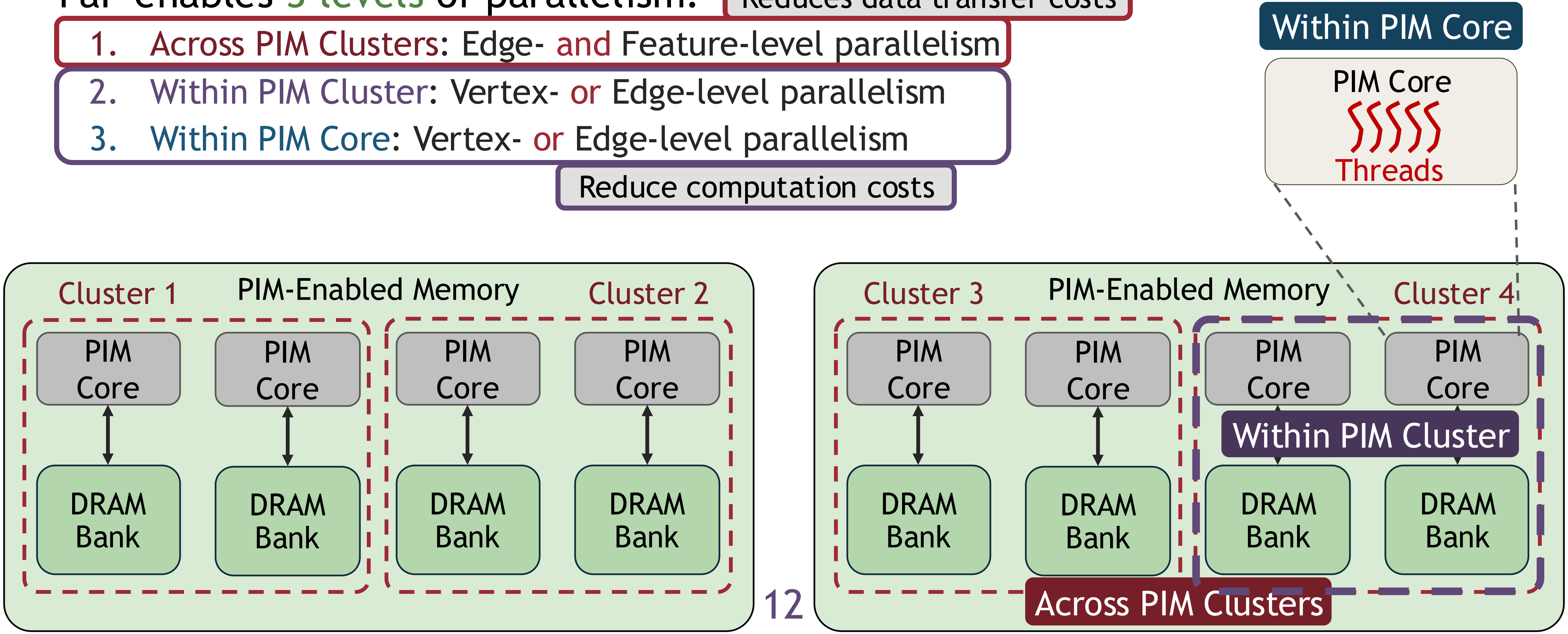


2. Parallelism Fusion (PaF)

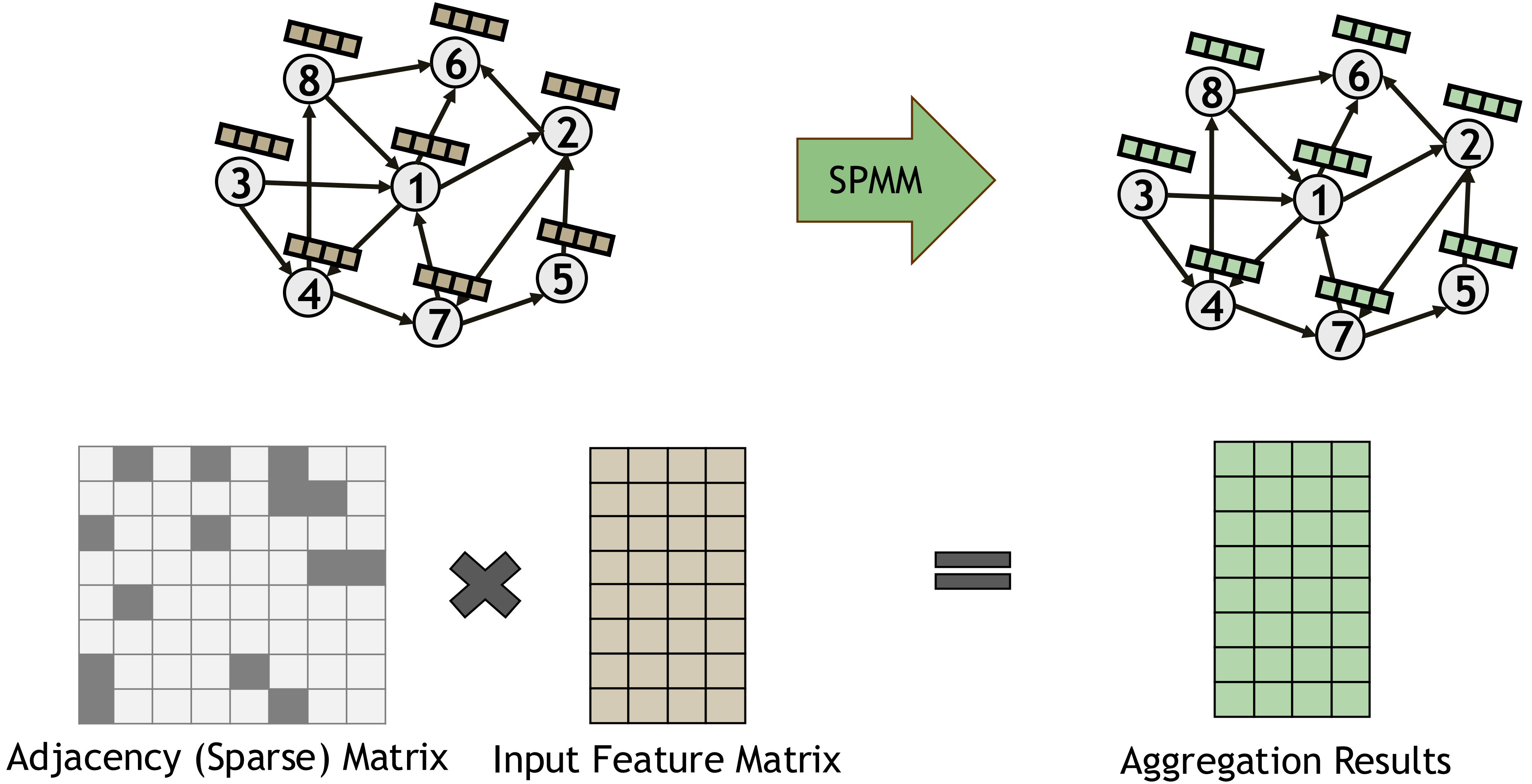
- PaF (i) strives a balance between *computation* and *data transfer* costs and
  (ii) covers various *graphs* with *diverse characteristics*
- PaF enables 3 levels of parallelism: Reduces data transfer costs
  1. Across PIM Clusters: Edge- and Feature-level parallelism
  2. Within PIM Cluster: Vertex- or Edge-level parallelism
  3. Within PIM Core: Vertex- or Edge-level parallelism

  Reduce computation costs



An Aggregation Example

- E.g., a graph with 8 vertices and 14 edges
  - SPMM is used for aggregation



2.1 PaF Parallelism Across PIM Clusters

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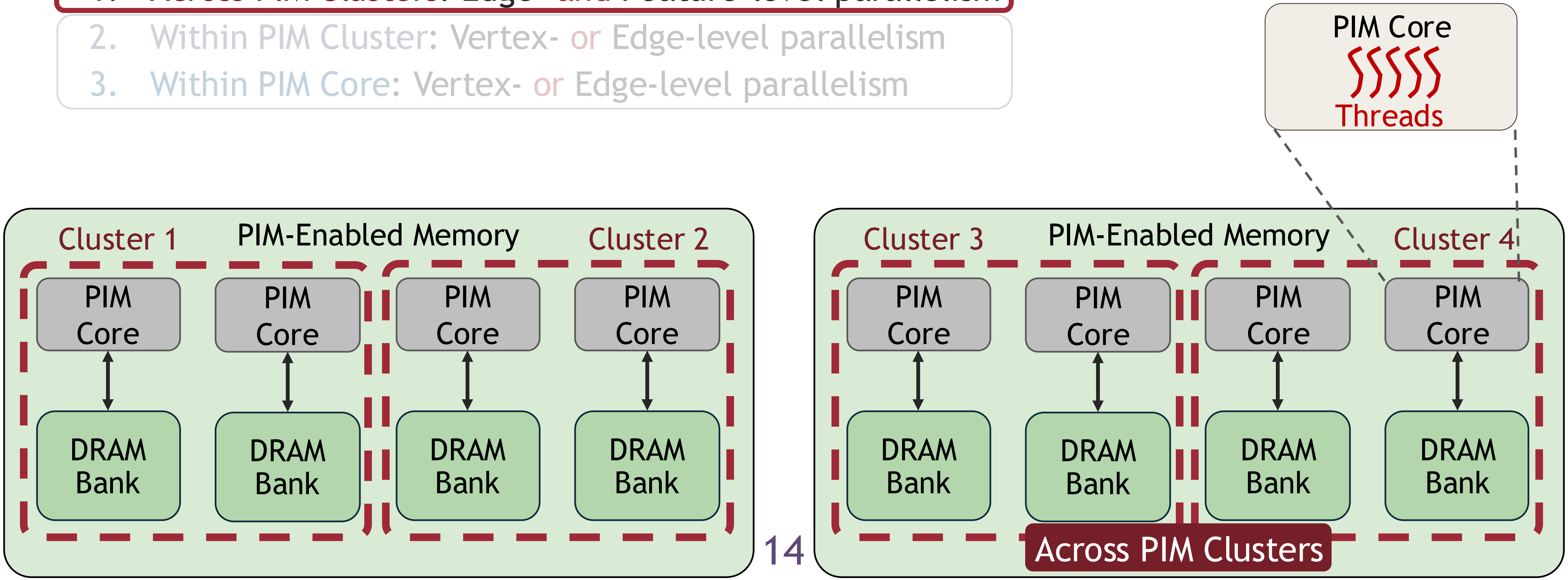
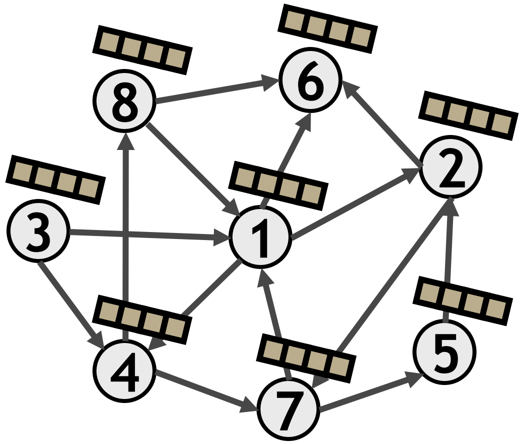
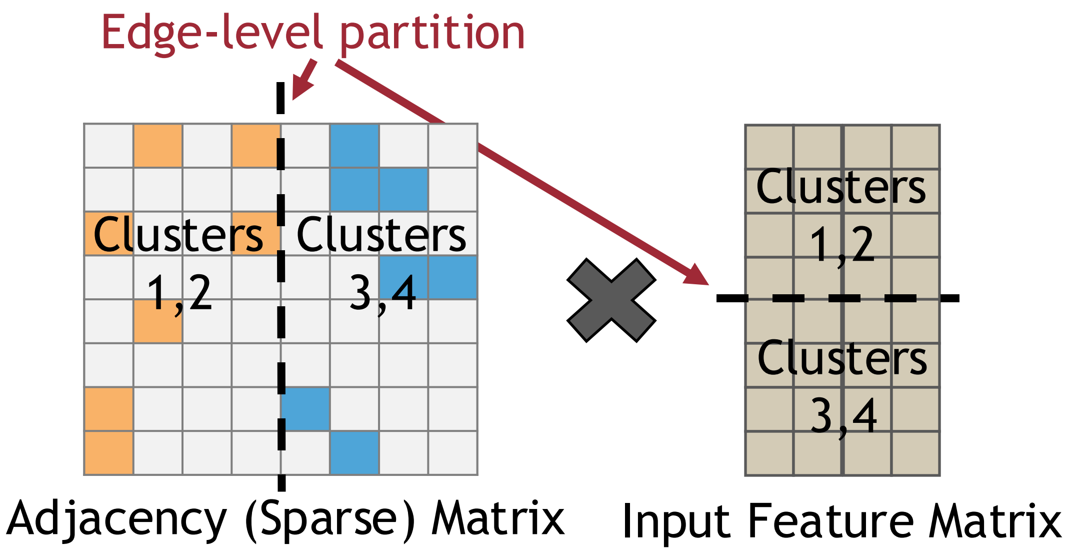


Across PIM Clusters: Edge- & Feature-Level Parallelism

- E.g., creating 4 PIM clusters with 2 Edge partitions and 2 Feature partitions





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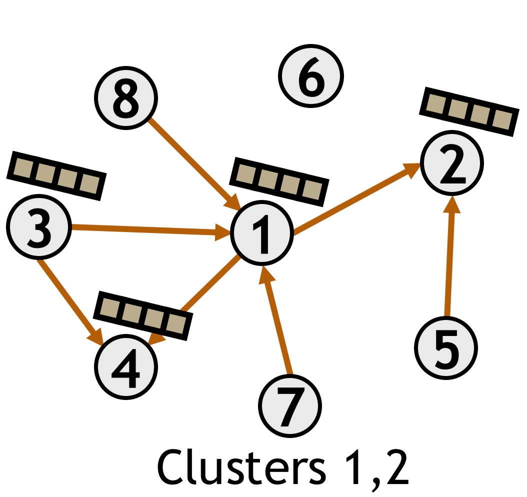

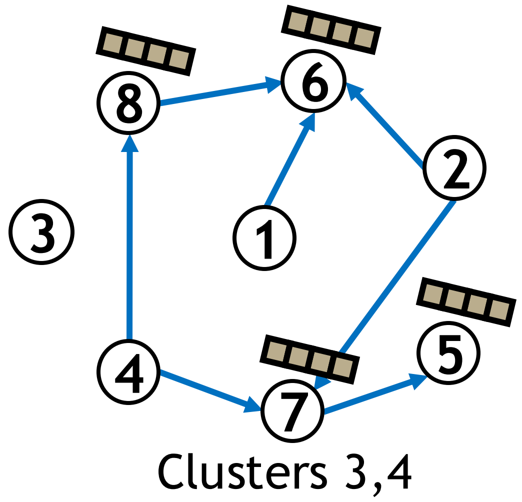

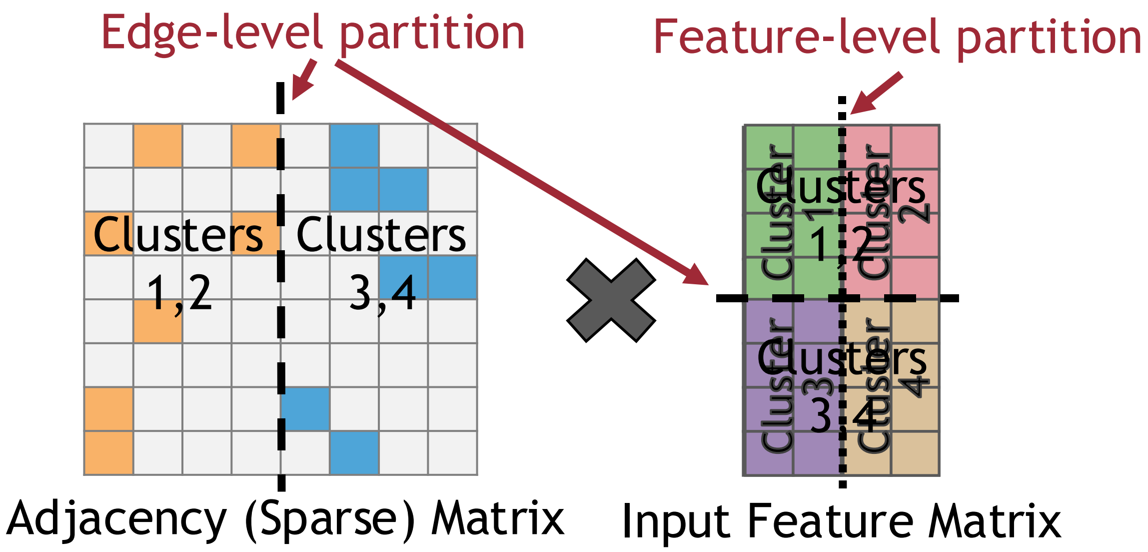

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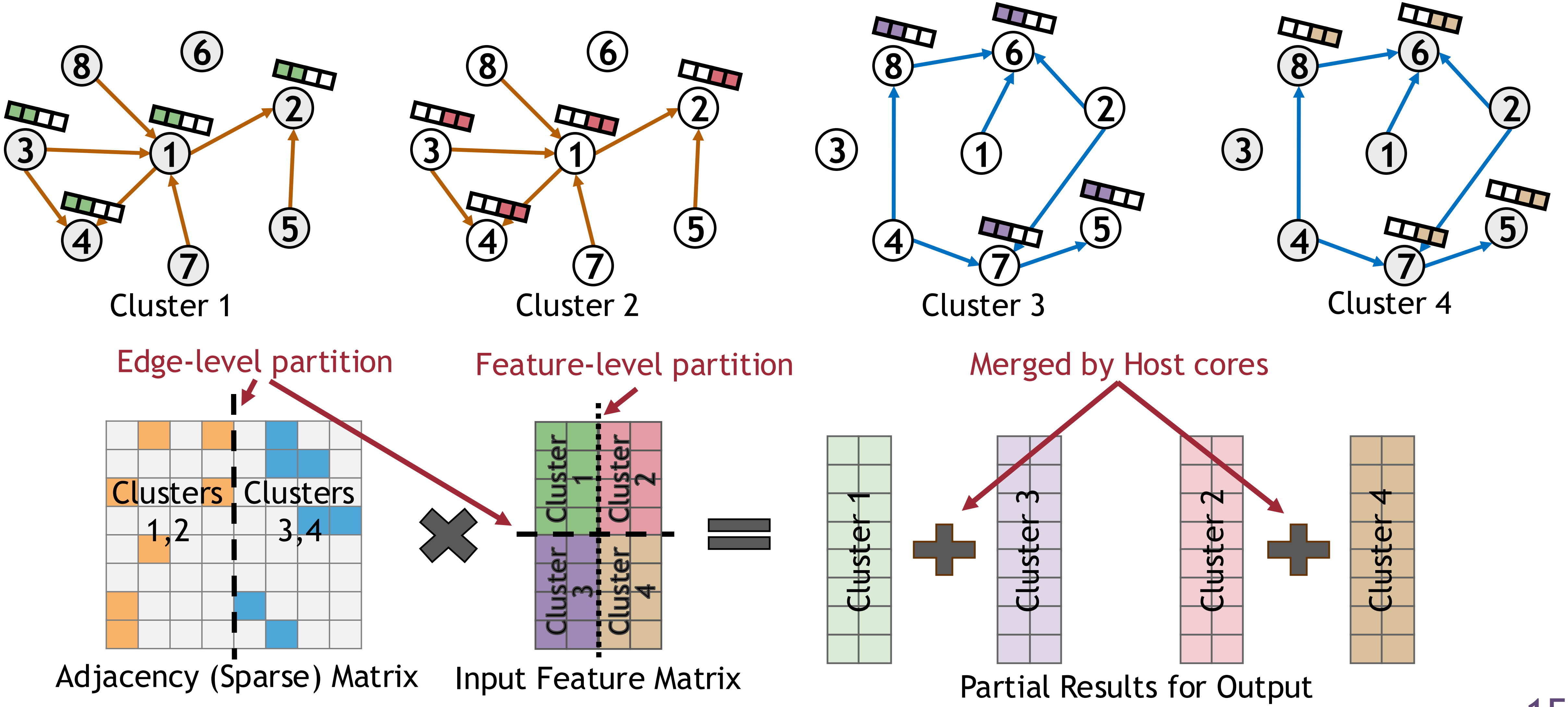

2.2 PaF Parallelism Within PIM Cluster

- PaF (i) strives a balance between *computation* and *data transfer* costs and
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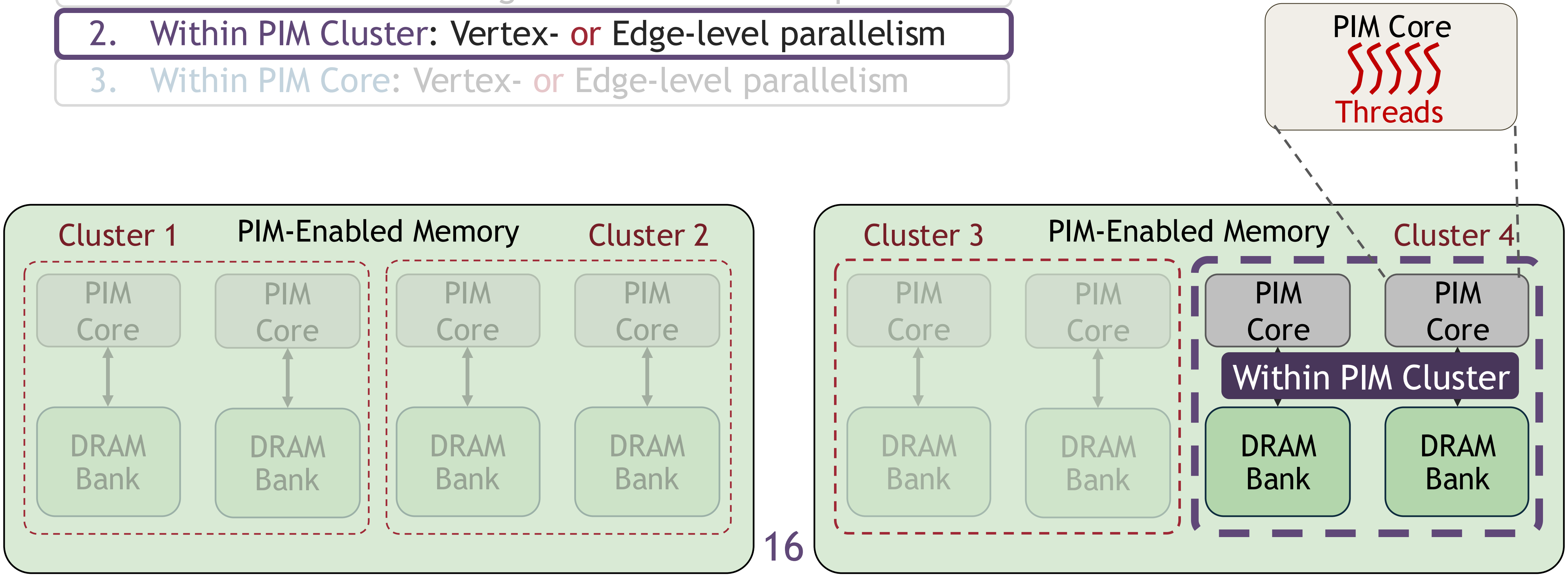
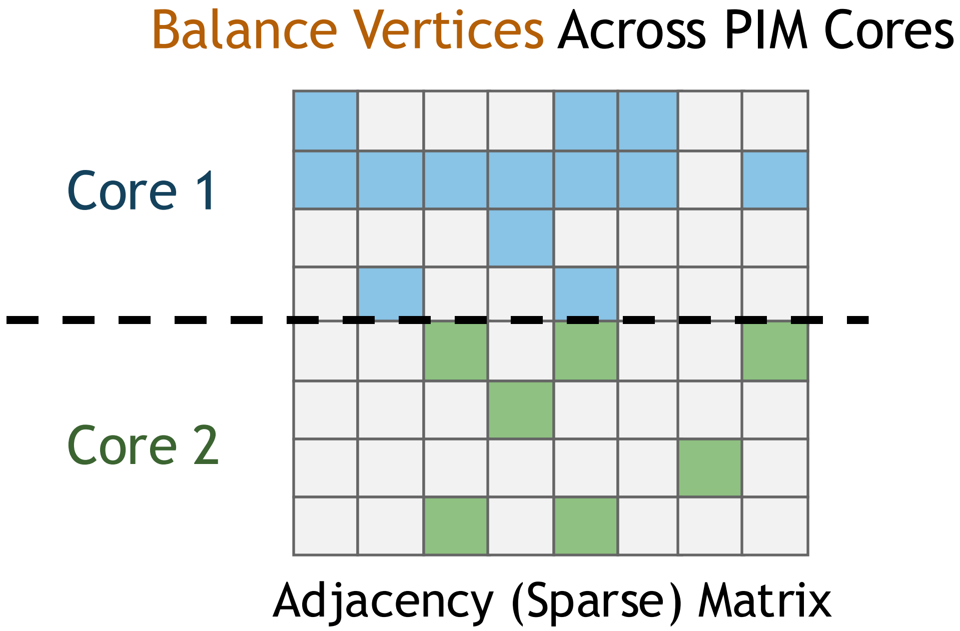
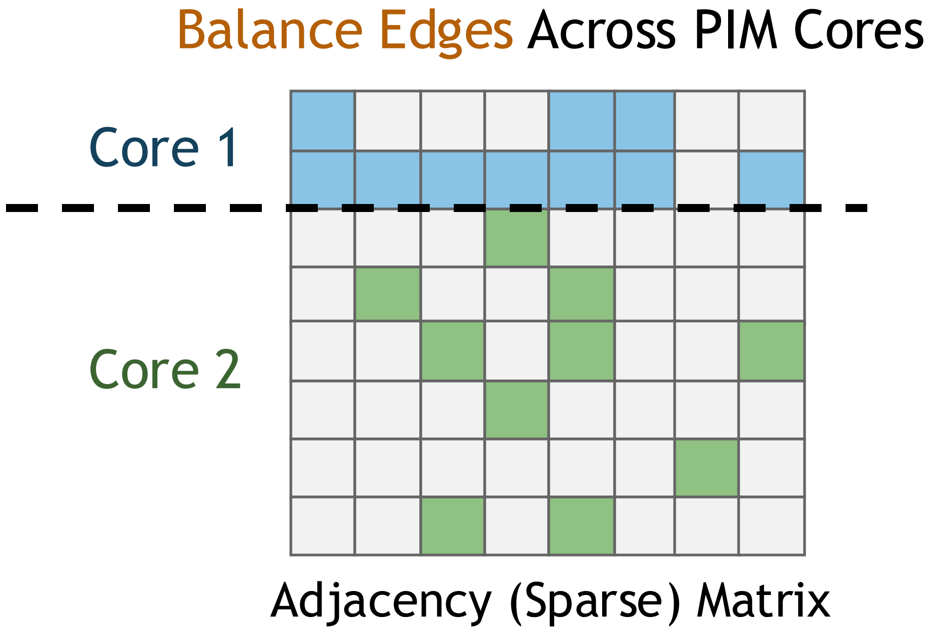
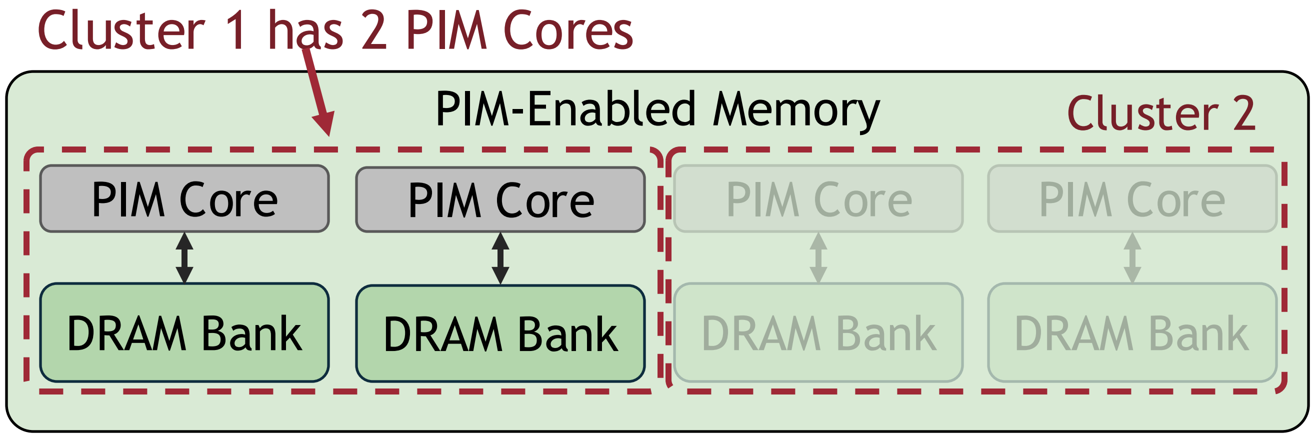


Within a PIM Cluster: Vertex- or Edge-Level Parallelism

- E.g., balancing vertices or balancing edges across PIM cores within the cluster







2.3 PaF Parallelism Within PIM Core

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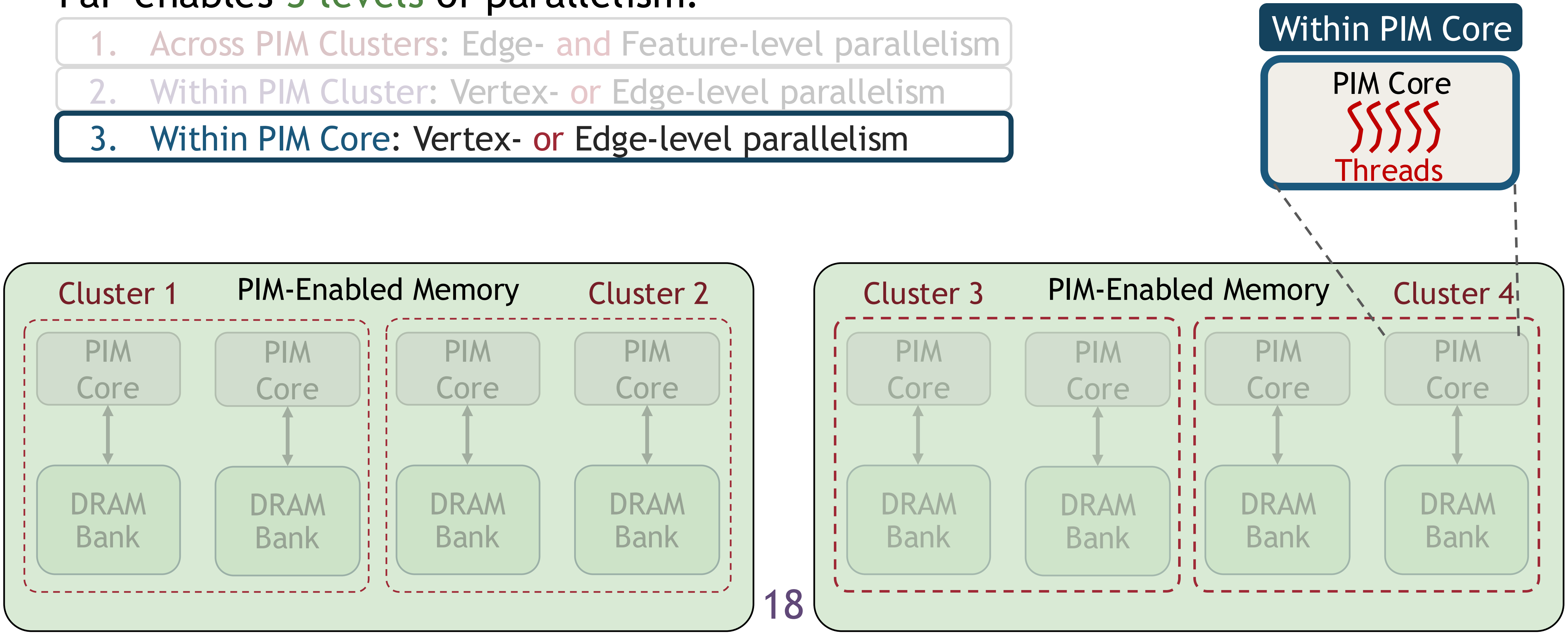
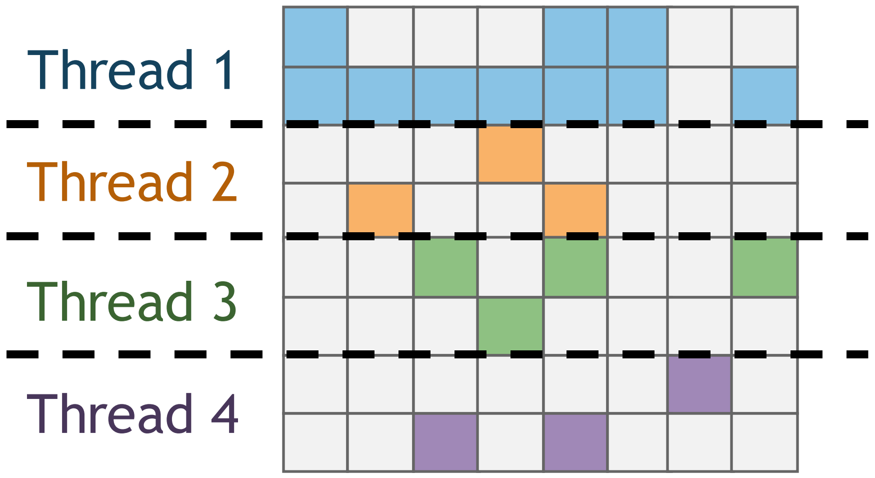


Within a PIM Core: Vertex- or Edge-Level Parallelism

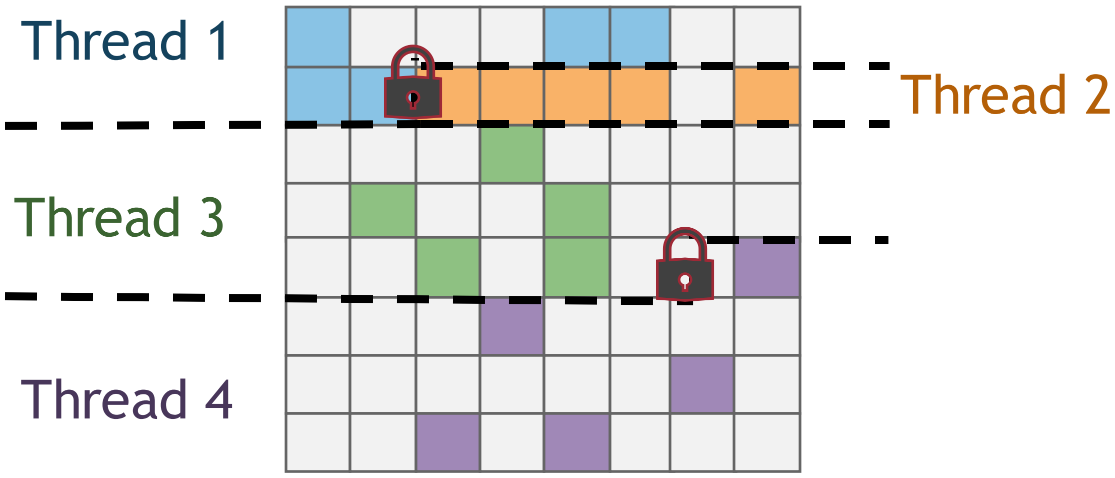
- E.g., balancing vertices or balancing edges across threads within a PIM core

Balance Vertices Across Threads



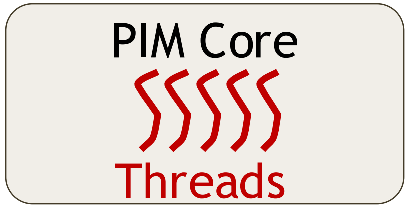
Adjacency (Sparse) Matrix

Balance Edges Across Threads



Adjacency (Sparse) Matrix

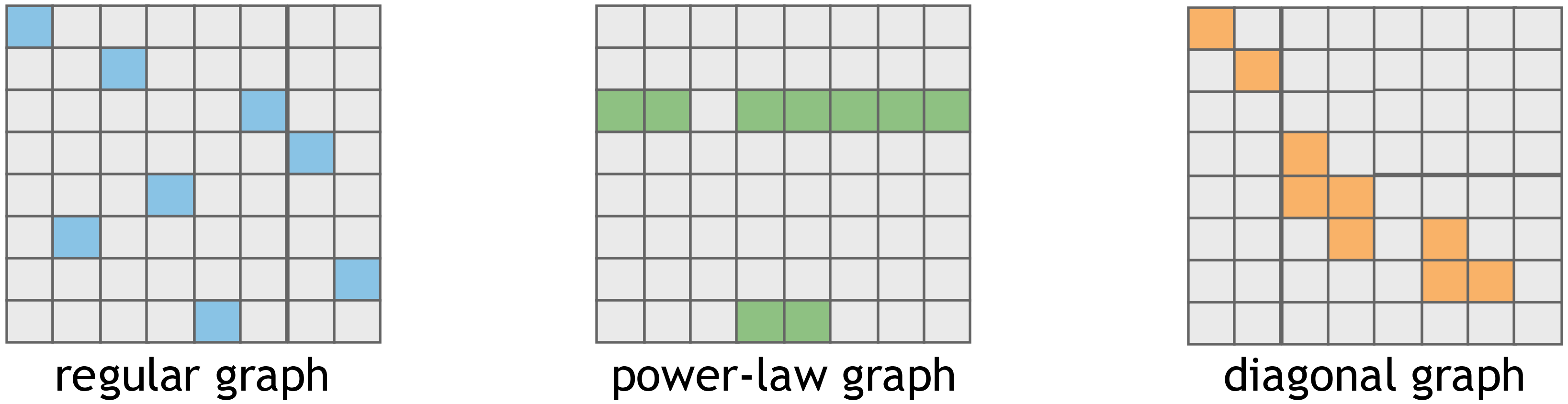
PIM Core supports
4 threads



Synchronization is implement
with lock-free or fine-grained locking schemes

Challenge 2: Programmability in Real-World Graphs

- PaF supports a wide variety of parallelization strategies:
  → Typically there is no one-size-fits-all solution
- Challenge = ***manually tuning*** the parallelization strategy poses significant burdens for developers
  - *Unique* graph's characteristics need different tuning



Real-world graphs exhibit diverse characteristics

PyGim Overview

- An efficient and easy-to-use GNN library for real PIM systems
- PyGim incorporates 4 key components:

Cooperative Acceleration (CoA)

Parallelism Fusion (PaF)

Lightweight Tuning

Handy Programming Interface

challenge

Expensive Data Transfer Costs

Programmability in
Real-World Graphs

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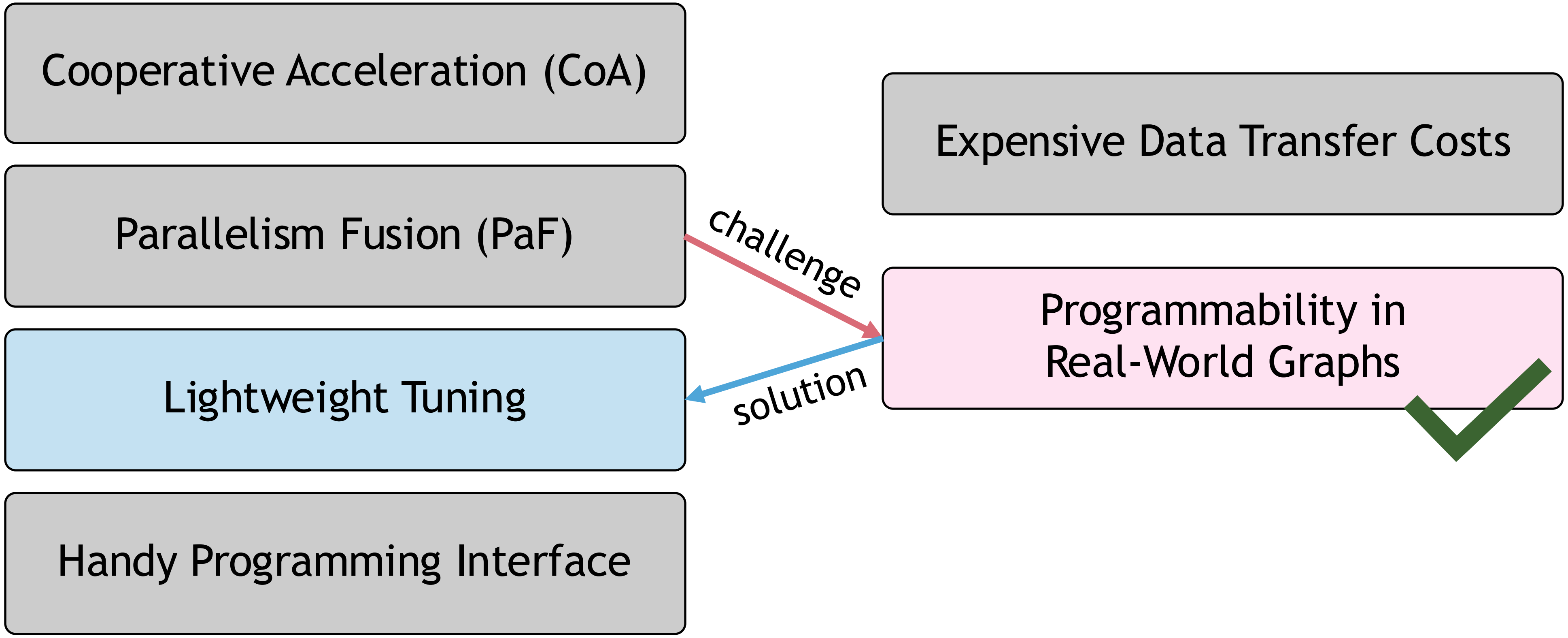
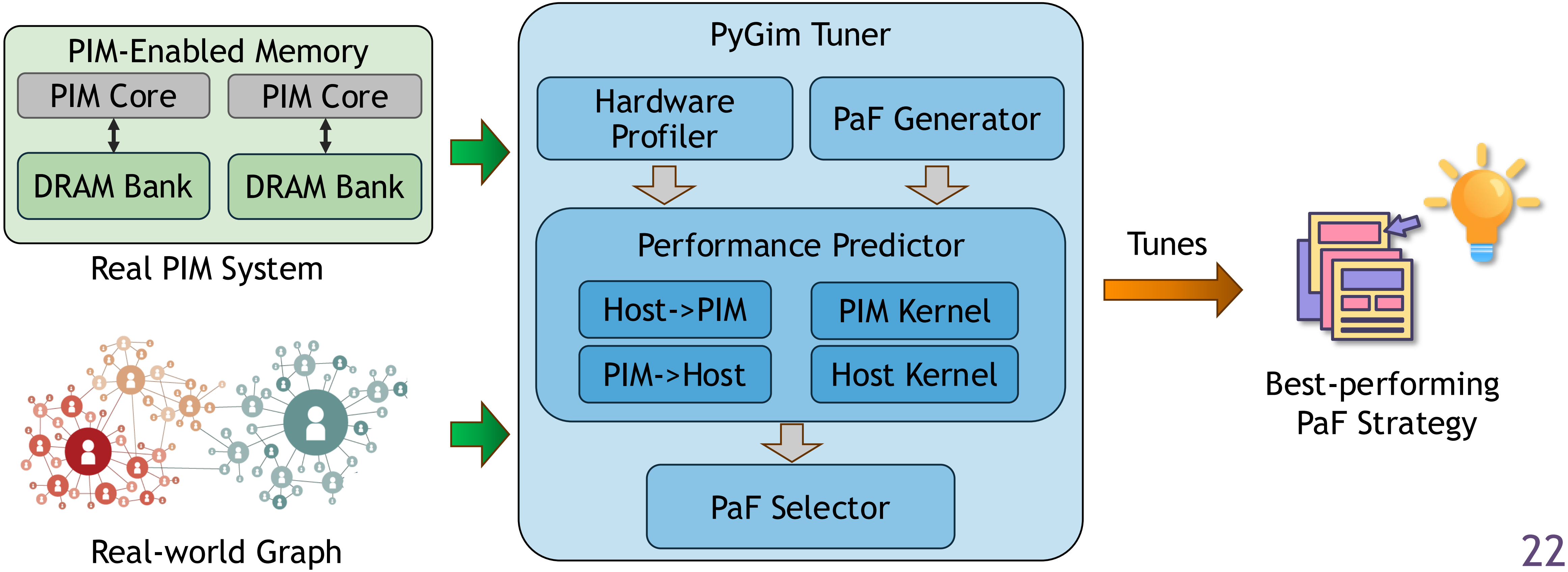


3. Lightweight Tuning

- PyGim Tuner predicts the *best-performing* PaF *strategy* without manual programmer intervention
  - Hardware profiler generate a group of performance measurements
  - Performance predictor predict the execution of potential PaF *strategy*
  - PaF selector apply the best-performing PaF strategy



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Handy Programming Interface

4. Handy Programming Interface

- PyGim integrates a *handy* Python API (currently integrated with PyTorch)

```
import …    pygim as gyn
class GCNConv(torch.nn.Module):
def __init__(self, hidden_size):
  self.linear = torch.nn.Linear(feature_size, features_size)

def forward(self, graph_pim, in_dense):
 # Execute memory-intensive kernel in real PIM devices
  dense_parts = col_split(in_dense)
 out_dense = gyn.pim_run_aggr(graph_pim, dense_parts)
  # Execute compute-intensive operator in Host (e.g., CPU/GPU)
  out = self.linear(out_dense)
  return out

gyn.pim_init_devices(num_pim_devices) # Initialize PIM devices
data = load_dataset() # Load graph
 # Tune the PaF strategy
graph_pim= gyn.tune(data.graph, feature_size, device_info)
graph_pim = gyn.load_graph_pim(graph_parts) # Partition graph to PIM
 # Create GNN model
 model=torch.nn.Sequential([Linear(in_channels,feature_size),
     GCNConv(feature_size),
     GCNConv(feature_size),
     GCNConv(feature_size),
     Linear(feature_size, out_channels)])
model.forward(graph_pim, data.features) # GCN inference
```

Deploy Your GNNs Effortlessly with PyGim and Enjoy the PIM Benefits!

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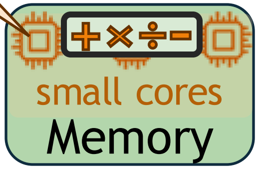
```

Computation is performed inside **real** PIM devices!

```
Loading kernel from: /home/upmem0013/
m_mul_coo_dpu
1000 DPUs are allocated in 16 ranks
Allocated 16 TASKLET(s) per DPU
BLNC = BLNC_NNZ
SYNC = True
BLNC_TSKLT = BLNC_TSKLT_NNZ
LOCK = LOCKFREEV2
MERGE = BLOCK
PIM_SEQREAD_CACHE_SIZE=32
val_dt = INT32
spmm_coo_to_device_group
prepare_pim finished


Iteration 0000:  Time: 7127.9930 ms.
Iteration 0001:  Time: 7191.6390 ms.
Iteration 0002:  Time: 7102.1040 ms.
Iteration 0003:  Time: 6888.6810 ms.
Iteration 0004:  Time: 7075.0290 ms.
Iteration 0005:  Time: 6844.8220 ms.
```

fast-forwarded



UPMEM PIM

Talk Outline

Background & Motivation

PyGim Design

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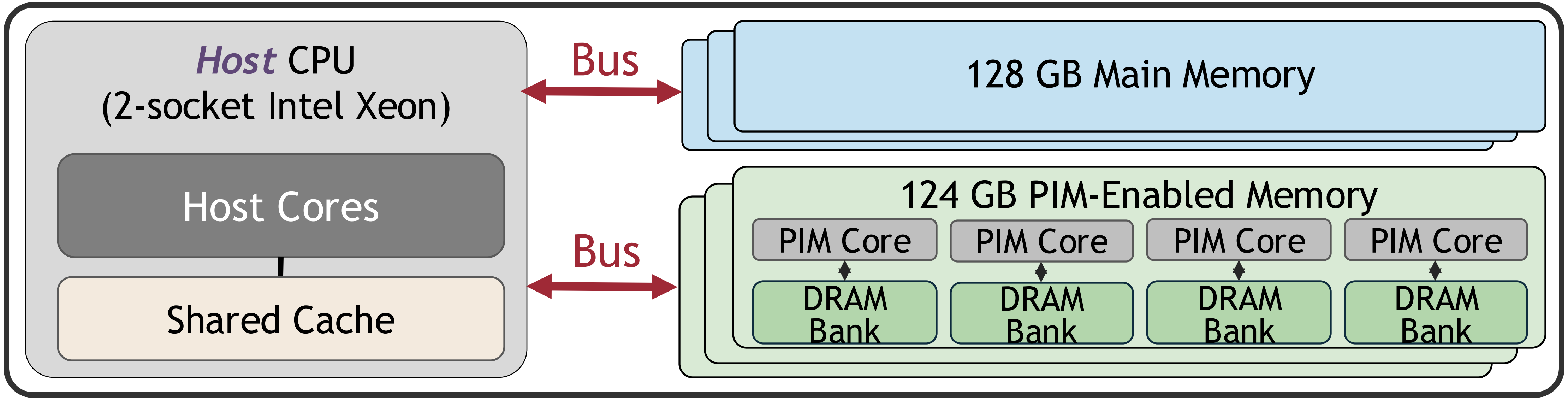
Evaluation Methodology

- UPMEM PIM server: 16 PIM DIMMs with *1992* PIM Cores (24 threads per core) in total
- GNN models: GCN, GIN, SAGE
- Datasets: OGBN-Proteins, Reddit, AmazonProducts
- Comparison points:
  - PyTorch running on host CPU
  - SparseP [Sigmetrics'22] (2×) running SpMM as multiple SpMV kernels on PIM cores
  - GraNDe [IEEE Trans. Comput.'23]: optimizes GNN aggregation on near-rank PIM systems

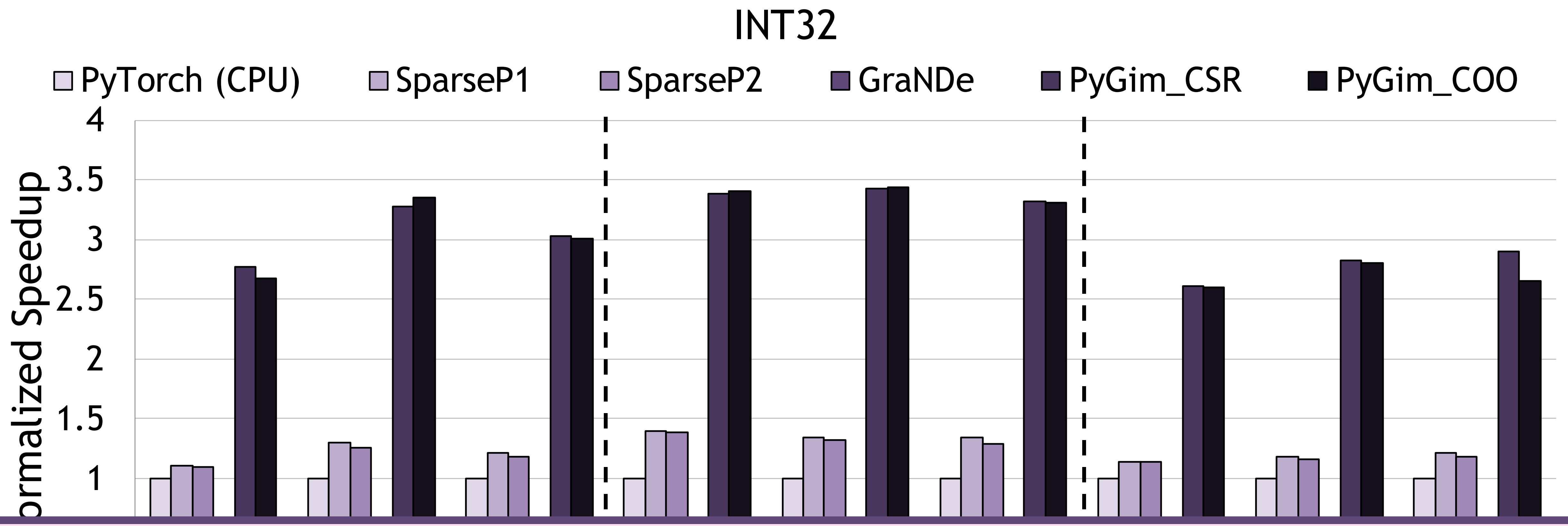


UPMEM PIM System

Performance Evaluation in GNN Inference

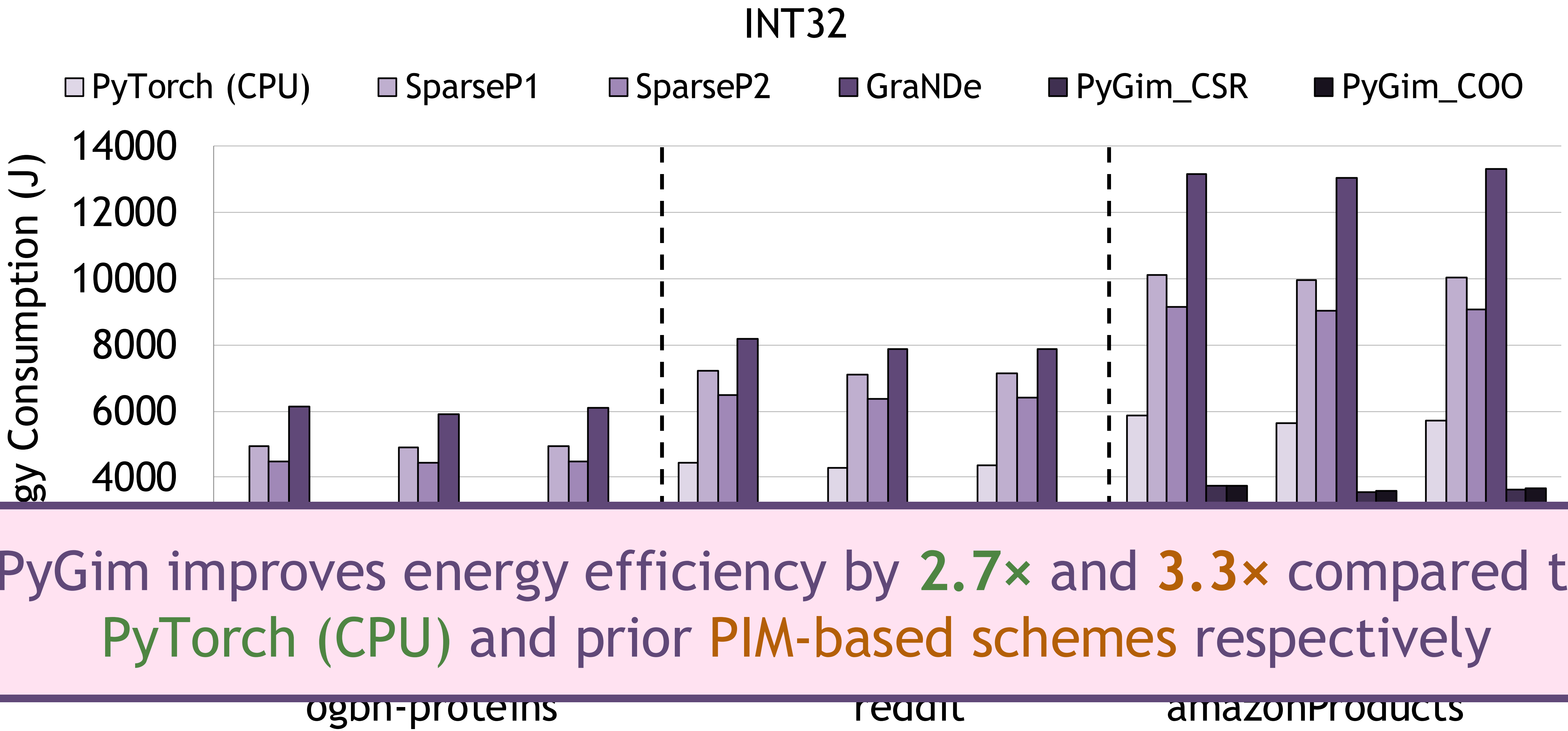
INT32

Performance Evaluation in GNN Inference



PyGim significantly outperforms PyTorch (CPU) and prior PIM-based schemes by 3.1× and 4.4× respectively

Energy Efficiency Evaluation in GNN Inference



PyGim improves energy efficiency by **2.7×** and **3.3×** compared to PyTorch (CPU) and prior PIM-based schemes respectively

Characteristics of CPU, PIM and GPU Systems

System	INT32 Peak Performance	FP32 Peak Performance	Total Bandwidth	Technology Node
CPU Xeon 4215	0.64 TOPS	1.28 TFLOPS	23.1 GB/s	14nm
UPMEM PIM	0.12 TOPS	0.025 TFLOPS	1390 GB/s	at least 20nm
GPU GTX 1080 Ti	13.25 TOPS	13.25 TFLOPS	359.9 GB/s	16nm
GPU RTX 2080 Ti	16.94 TOPS	16.94 TFLOPS	558.1 GB/s	12nm
GPU RTX 3090	17.79 TOPS	35.58 TFLOPS	936.2 GB/s	8nm

Across last GPU generations:

- *memory bandwidth* has tripled (~**3×**)
- (last two generations) *compute throughput* has been doubled (~**2×**)

Core Utilization in GNN Aggregation

Dataset & data type/ Software library	Reddit INT32	Reddit FP32
Intel MKL (CPU Intel Xeon 4215)	0.63%	0.22%
CUDA (GPU GTX 1080 Ti)	0.62%	0.62%
CUDA (GPU RTX 2080 Ti)	0.68%	0.67%
CUDA (GPU RTX 3090)	1.56%	0.78%
PyGim (UPMEM PIM)	**13.86%**	**9.13%**

Core utilization in GNN aggregation remains *similarly low* across GPU generations

PyGim running on a real PIM system achieves
significantly higher core utilization(11.6x on average) than the PyTorch on GPUs

More in the Paper

- Analysis within a PIM core
- Analysis within a PIM cluster
- Analysis across PIM clusters
- PyGim tuning efficiency
- Scalability analysis
- Analysis on different data types
- Analysis on different compression formats
- Performance evaluation in GNN training
- Recommendations

PyGim: An Efficient Graph Neural Network Library for Real Processing-In-Memory Architectures

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Graph Neural Networks (GNNs) are emerging models to analyze graph-structure data. The GNN execution involves both compute-intensive and memory-intensive kernels. The memory-intensive kernels dominate execution time, because they are significantly bottlenecked by data movement between memory and processors. Processing-In-Memory (PIM) systems can alleviate this data movement bottleneck by placing simple processors near or inside memory arrays. To this end, we investigate the potential of PIM systems to alleviate the data movement bottleneck in GNNs, and introduce PyGim, an efficient and easy-to-use GNN library for real PIM systems. We propose intelligent parallelization techniques for memory-intensive kernels of GNNs tailored for real PIM systems, and develop an easy-to-use Python API for them. PyGim employs a cooperative GNN execution, in which the compute- and memory-intensive kernels are executed in processor-centric and memory-centric computing systems, respectively, to fully exploit the hardware capabilities. PyGim integrates a lightweight tuner that configures the parallelization strategy of the memory-intensive kernel of GNNs to provide high system performance, while also enabling high programming ease. We extensively evaluate PyGim on a real-world PIM system that has 16 PIM DIMMs with 1992 PIM cores connected to a Host CPU. In GNN inference, we demonstrate that it outperforms prior state-of-the-art PIM works by on average 4.38× (up to 7.20×), and the state-of-the-art PyTorch implementation running on Host (on Intel Xeon CPU) by on average 3.04× (up to 3.44×). PyGim improves energy efficiency by 2.86× (up to 3.68×) and 1.55× (up to 1.75×) over prior PIM and PyTorch Host schemes, respectively. In memory-intensive kernel of GNNs, PyGim provides 11.6× higher resource utilization in PIM system than that of PyTorch library (optimized CUDA implementation) in GPU systems. Our work provides useful recommendations for software, system and hardware designers. PyGim is publicly and freely available at https://github.com/CMU-SAFARI/PyGim to facilitate the widespread use of PIM systems in GNNs.

Key Words: machine learning, graph neural networks, sparse matrix-matrix multiplication, library, multicore, processing-in-memory, near-data processing, memory systems, data movement bottleneck, DRAM, benchmarking, real-system characterization, workload characterization

https://arxiv.org/pdf/2402.16731

Conclusion

We present ***PyGim***, a handy ML library that significantly improves *performance*, *energy efficiency* and *cost effectiveness* in GNNs through real PIM devices

Key Ideas & Benefits:

- *balances computation* and *data transfer* costs via configurable parallelization strategies for *diverse* real-world graphs
- *automatically* tunes the best-fit strategy *without programmer intervention*

Key Results:

- *performance* and *energy efficiency* by 3.7× and 2.3× over SOTA schemes
- *core utilization* on PIM system by 11.6× over PyTorch on GPUs

PyGim

Github

Paper

PyGim: An Efficient Graph Neural Network Library for Real Processing-In-Memory Architectures

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