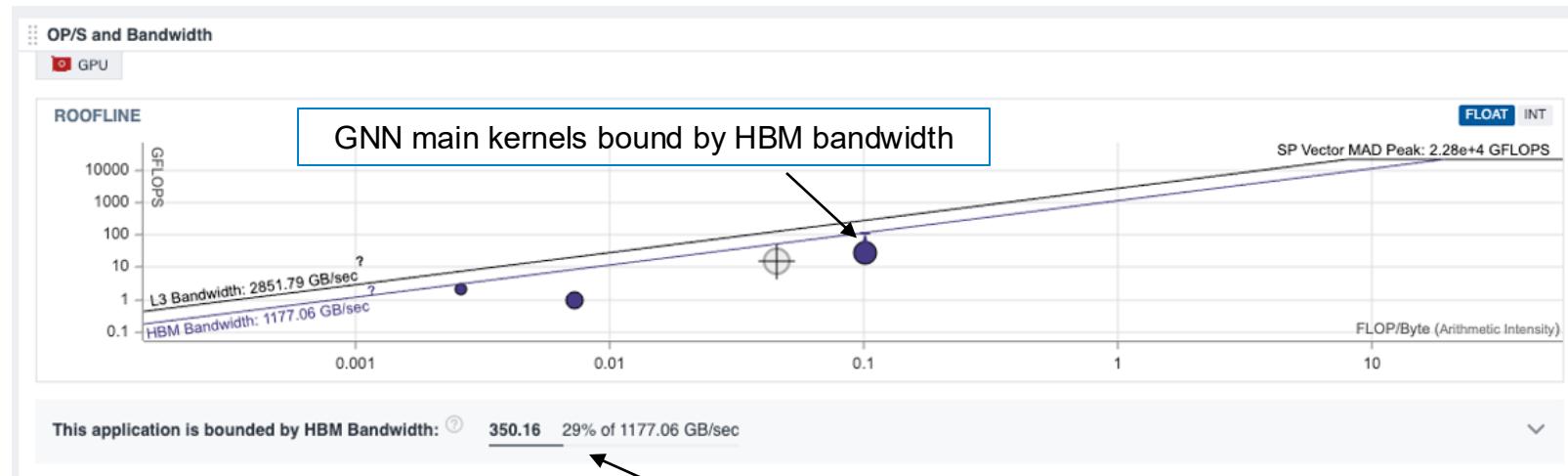


DIST-GNN: OVERVIEW

- Dist-GNN model for mesh-based modeling of dynamical systems
 - Operates on partitions of the entire graph, called sub-graphs, created directly from the CFD mesh used by nekRS
 - Size of sub-graph determined by nekRS mesh size and by polynomial order used to create GNN graph (this is \leq p-order used by nekRS)
 - Implements a halo exchange in the neural message passing layers to ensure node aggregation steps span across sub-graphs, thereby enabling training and inference on extremely large graphs
- Implemented in PyTorch and PyTorch Geometric
- Run with FP32 or BF16 (FP16 or lower not suitable for science needs)

ROOFLINE (FP32)

- Dist-GNN training roofline collected with Intel Advisor on single Aurora PVC tile
 - GNN main kernels are **HMB bandwidth bound** (even GEMM)
 - Dist-GNN application as a whole is also **HBM bandwidth bound**

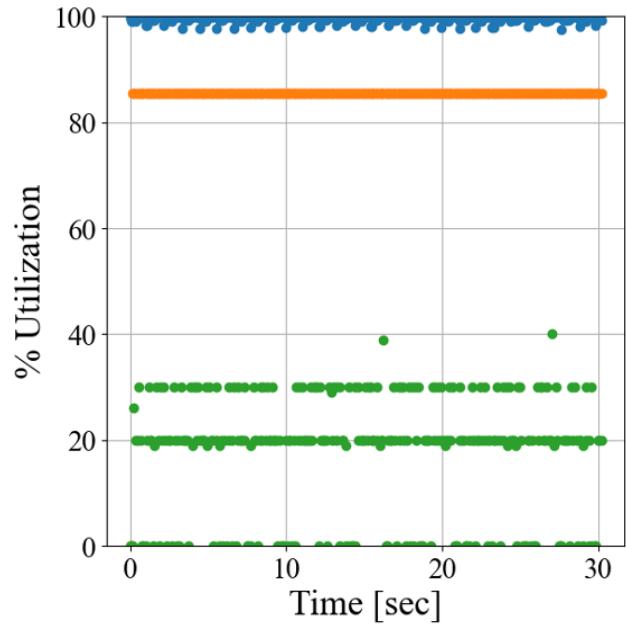


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GPU UTILIZATION ON AURORA

- GNN training GPU utilization metrics
 - Collected with xpu-smi on single PVC tile of Aurora
 - Note high (~85%) GPU memory utilization
 - Problem and model size for GNN **bound by GPU HBM memory size**



- GPU Utilization (%)
- GPU Memory Utilization (%)
- GPU Memory Bandwidth Utilization (%)