GPU Resource Partitioning and Bandwidth Analysis on SDumont II HPC Cluster

Pablo Alessandro Santos Hugen

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Abstract: This report measures CPU-GPU bandwidth and application performance on SDumont II's NVIDIA GH200 nodes, comparing exclusive and shared queue allocation modes. Using nvbandwidth, we measured 411 GB/s host-to-device bandwidth for local GPU access versus 88 GB/s for remote access (4.6x difference). In shared queue mode, SLURM's GRES scheduling maintained NUMA locality. GROMACS benchmarks (STMV, ~1M atoms) showed identical single-GPU performance in both queues (43.45 ns/day). Multi-GPU scaling achieved 2.5x speedup with 4 GPUs; 2-GPU runs showed no benefit due to communication overhead.

Keywords: GPU partitioning, NUMA, NVLink, SLURM, HPC, SDumont II, GROMACS

0.1 1. Introduction

0.1.1 1.1 Motivation

SDumont II at LNCC offers two allocation modes for NVIDIA GH200 nodes: - **Exclusive queue**: Full node reserved for one job - **Shared queue**: SLURM GRES scheduling partitions resources among jobs

This work measures: 1. CPU-GPU bandwidth under different NUMA configurations 2. Whether SLURM preserves NUMA locality in shared mode 3. Application performance differences between queues

0.1.2 1.2 GH200 Node Architecture

Each SDumont II node contains four GH200 superchips: - 72 Arm Neoverse V2 CPU cores per superchip - 120 GB HBM3 GPU memory per GPU - NVLink-C2C: 900 GB/s CPU-GPU bandwidth (local) - NVLink 4.0 between GPUs

0.1.3 1.3 NUMA Topology

GPU-NUMA affinity: - GPU 0   NUMA 0 (cores 0-71) - GPU 1   NUMA 1 (cores 72-143) - GPU 2   NUMA 2 (cores 144-215) - GPU 3   NUMA 3 (cores 216-287)

0.2 2. Experimental Setup

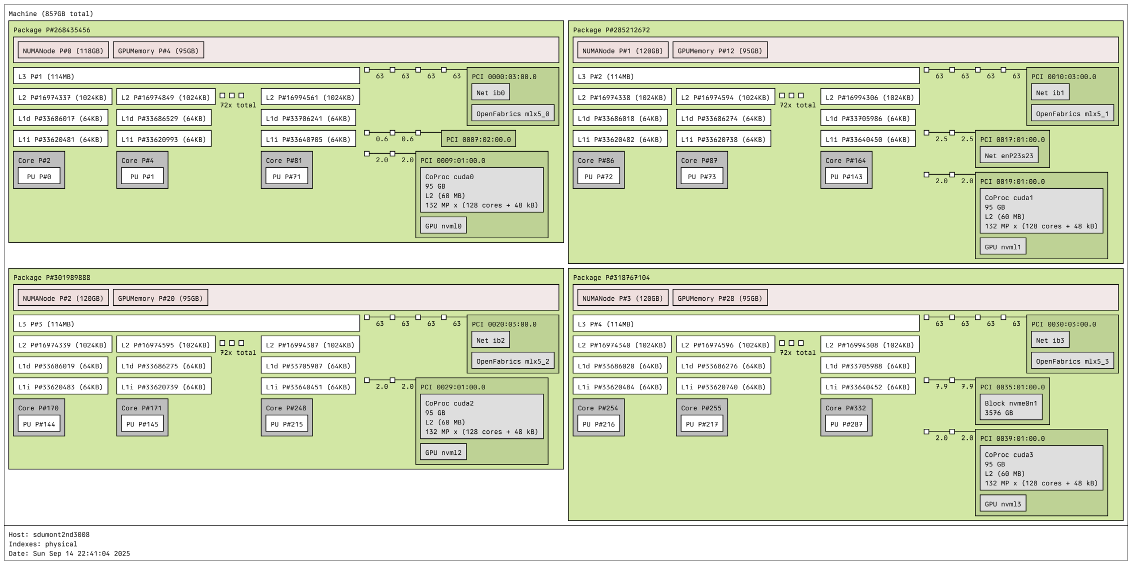
0.2.1 2.1 Hardware Configuration

```
[1]: import pandas as pd, numpy as np, matplotlib.pyplot as plt, seaborn as sns, re,␣
       ↪warnings
     from pathlib import Path
     warnings.filterwarnings('ignore')
     plt.style.use('seaborn-v0_8-whitegrid')
     plt.rcParams.update({'figure.figsize': (12, 6), 'font.size': 11, 'axes.
       ↪titlesize': 14, 'axes.labelsize': 12})
     RESULTS_DIR = Path('../../data/transfer')
```

Hardware Specifications

Component	Specification
Node Type	NVIDIA GH200 Grace Hopper Superchip
GPUs per Node	4x NVIDIA GH200 120GB
GPU Memory	120 GB HBM3 per GPU
CPU Cores	288 (72 per NUMA package)
CPU Memory	~480 GB LPDDR5X (120 GB per package)
GPU Interconnect	NVLink 4.0 (NV6 = 6 NVLinks bonded)
CUDA Version	12.6
Driver Version	560.35.03

Node Topology The following diagram illustrates the topology of a GH200 node:



Key observations: - 4 NVIDIA GH200 GPUs per node - 4 CPU NUMA packages (0-3) - Each GPU has affinity to one NUMA package - All GPUs connected via NVLink 4.0 (NV6 = 6 bonded links)

0.2.2 2.2 Queue Configurations

Queue	Type	Description	Max GPUs
`gh200`	Exclusive	Full node reserved for a single job	4
`gh200_shared`	Shared	GRES scheduling among multiple jobs	2

0.2.3 2.3 Tools and Methodology

Tool	Version	Purpose
numactl	-	NUMA scheduling policy management
nvbandwidth	v0.6	CPU-GPU and GPU-GPU bandwidth measurement
nvidia-smi	560.35.03	GPU topology and monitoring

0.3 3. Experiments

0.3.1 3.1 Bandwidth Benchmarks (nvbandwidth)

Exclusive Queue

- Pin process to each NUMA (0-3) using `numactl --cpunodebind --membind`
- Measure bandwidth to all 4 GPUs per pinning
- Result: 4×4 bandwidth matrix

Shared Queue

- Submit concurrent jobs requesting 1 or 2 GPUs
- Observe SLURM's NUMA-GPU assignment
- Measure bandwidth to allocated GPUs

[2]:
```
def parse_h2d_bandwidth(filepath):
    with open(filepath, 'r') as f: content = f.read()
    match = re.search(r'Running host_to_device_memcpy_ce\.\nmemcpy CE␣
↪CPU\(row\) -> GPU\(column\) bandwidth \(GB/s\)\n\s+[\d\s]+\n\s*0\s+([\d\.
↪\s]+)\n', content)
    return [float(x) for x in match.group(1).strip().split()] if match else None

def parse_d2h_bandwidth(filepath):
    with open(filepath, 'r') as f: content = f.read()
    match = re.search(r'Running device_to_host_memcpy_ce\.\nmemcpy CE␣
↪CPU\(row\) <- GPU\(column\) bandwidth \(GB/s\)\n\s+[\d\s]+\n\s*0\s+([\d\.
↪\s]+)\n', content)
    return [float(x) for x in match.group(1).strip().split()] if match else None

def parse_latency(filepath):
    with open(filepath, 'r') as f: content = f.read()
    match = re.search(r'Running host_device_latency_sm\.\nmemory latency SM␣
↪CPU\(row\) <-> GPU\(column\) \(ns\)\n\s+[\d\s]+\n\s*0\s+([\d\.\s]+)\n',␣
↪content)
    return [float(x) for x in match.group(1).strip().split()] if match else None

def parse_numa_pinning(filepath):
    with open(filepath, 'r') as f: content = f.read()
    match = re.search(r'PINNED to (\d+)', content) or re.search(r'cpubind:␣
↪(\d+)\s*\n', content)
    return int(match.group(1)) if match else None
```

[3]:
```
exclusive_h2d, exclusive_d2h, exclusive_latency = {}, {}, {}
for i in range(4):
    filepath = RESULTS_DIR / f'exclusive_4gpu_node{i}.txt'
    if filepath.exists():
        numa = parse_numa_pinning(filepath)
        if (h2d := parse_h2d_bandwidth(filepath)): exclusive_h2d[numa] = h2d
        if (d2h := parse_d2h_bandwidth(filepath)): exclusive_d2h[numa] = d2h
        if (lat := parse_latency(filepath)): exclusive_latency[numa] = lat

h2d_df = pd.DataFrame(exclusive_h2d, index=[f'GPU {i}' for i in range(4)]).T
h2d_df.index, h2d_df.columns = [f'NUMA {i}' for i in h2d_df.index], [f'GPU {i}'␣
↪for i in range(4)]
d2h_df = pd.DataFrame(exclusive_d2h, index=[f'GPU {i}' for i in range(4)]).T
d2h_df.index, d2h_df.columns = [f'NUMA {i}' for i in d2h_df.index], [f'GPU {i}'␣
↪for i in range(4)]
latency_df = pd.DataFrame(exclusive_latency, index=[f'GPU {i}' for i in␣
↪range(4)]).T
latency_df.index, latency_df.columns = [f'NUMA {i}' for i in latency_df.index],␣
↪[f'GPU {i}' for i in range(4)]

local_h2d = [h2d_df.iloc[i, i] for i in range(4)]
remote_h2d = [h2d_df.iloc[i, j] for i in range(4) for j in range(4) if i != j]
local_lat = [latency_df.iloc[i, i] for i in range(4)]
remote_lat = [latency_df.iloc[i, j] for i in range(4) for j in range(4) if i !=␣
↪j]
```

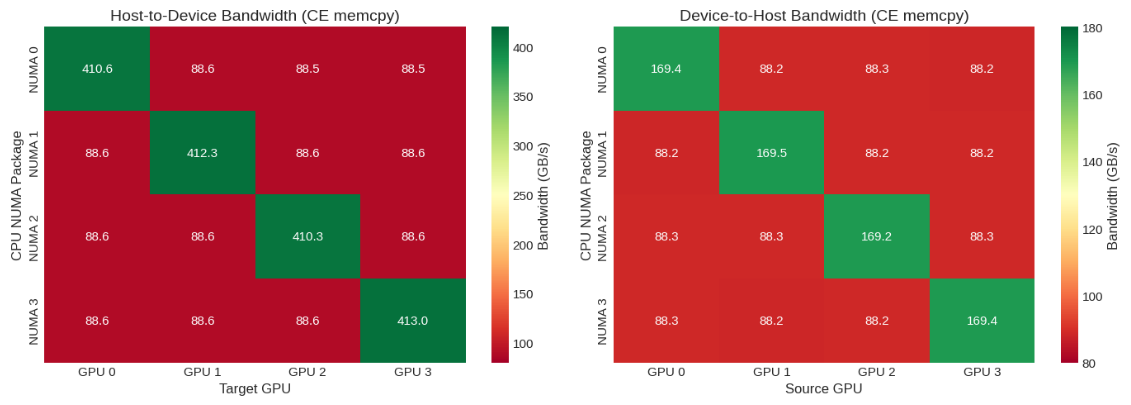
0.4 4. Results and Discussion

0.4.1 4.1 Bandwidth Results

4.1.1 Exclusive Queue - Host-to-Device Bandwidth

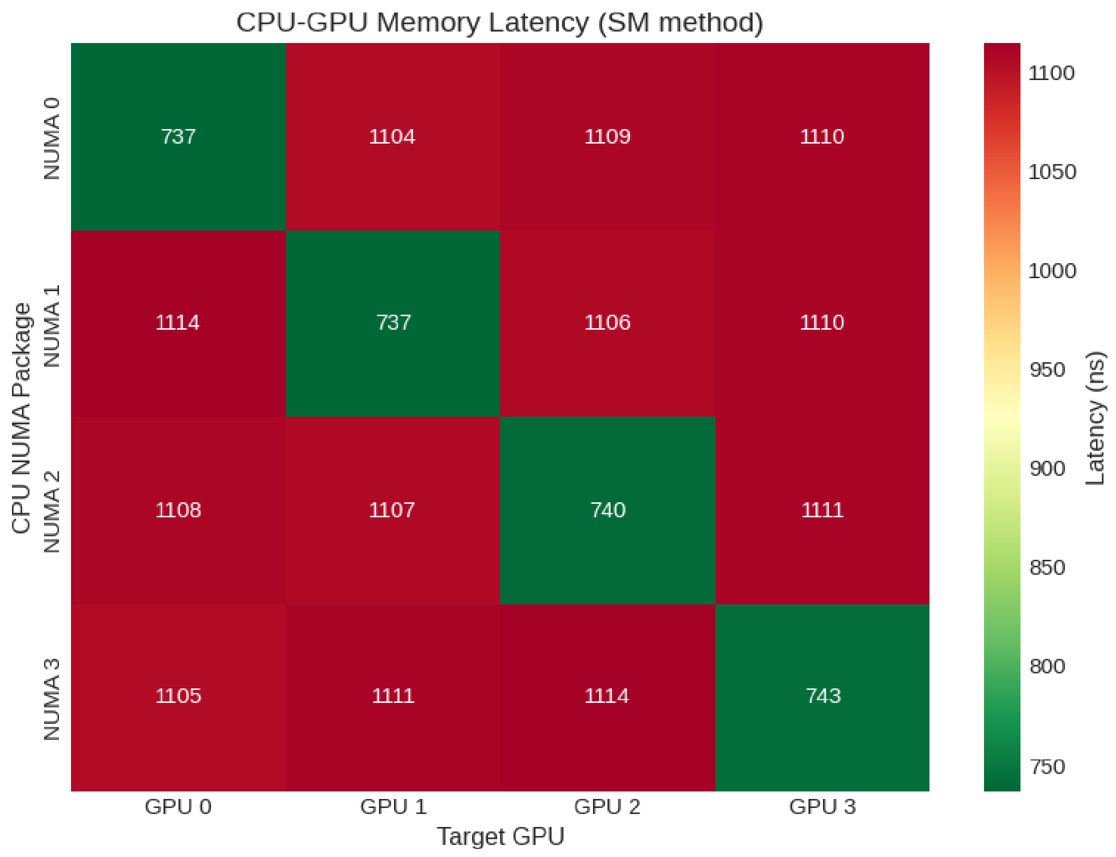
[4]:
```
fig, axes = plt.subplots(1, 2, figsize=(14, 5))
sns.heatmap(h2d_df, annot=True, fmt='.1f', cmap='RdYlGn', ax=axes[0], vmin=80,␣
↪vmax=420, cbar_kws={'label': 'Bandwidth (GB/s)'})
```

```
axes[0].set_title('Host-to-Device Bandwidth (CE memcpy)'); axes[0].
  ↪set_xlabel('Target GPU'); axes[0].set_ylabel('CPU NUMA Package')
sns.heatmap(d2h_df, annot=True, fmt='.1f', cmap='RdYlGn', ax=axes[1], vmin=80,␣
  ↪vmax=180, cbar_kws={'label': 'Bandwidth (GB/s)'})
axes[1].set_title('Device-to-Host Bandwidth (CE memcpy)'); axes[1].
  ↪set_xlabel('Source GPU'); axes[1].set_ylabel('CPU NUMA Package')
plt.tight_layout(); plt.savefig('img/bandwidth_heatmaps.png', dpi=150,␣
  ↪bbox_inches='tight'); plt.show()
```



Result: Local GPU access (diagonal) achieves ~410 GB/s; remote access (off-diagonal) achieves ~88 GB/s. This 4.6x difference reflects NVLink-C2C (local) versus inter-socket interconnect (remote).

[5]:
```
fig, ax = plt.subplots(figsize=(8, 6))
sns.heatmap(latency_df, annot=True, fmt='.0f', cmap='RdYlGn_r', ax=ax,␣
  ↪cbar_kws={'label': 'Latency (ns)'})
ax.set_title('CPU-GPU Memory Latency (SM method)'); ax.set_xlabel('Target GPU');
  ↪ ax.set_ylabel('CPU NUMA Package')
plt.tight_layout(); plt.savefig('img/latency_heatmap.png', dpi=150,␣
  ↪bbox_inches='tight'); plt.show()
```

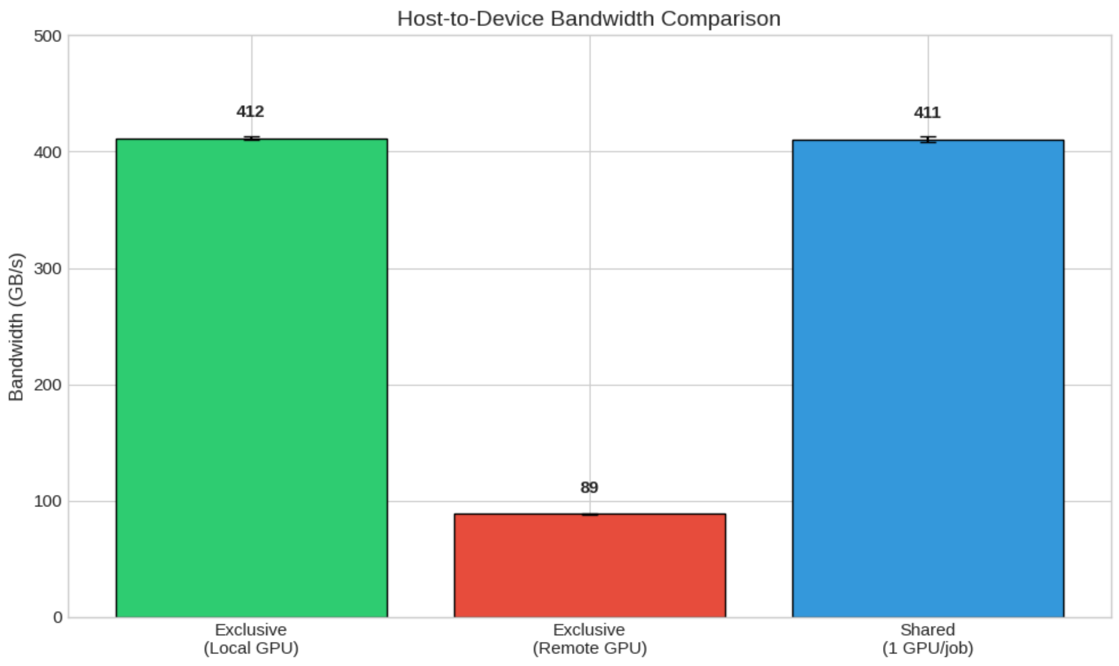


Latency: Local ~737 ns, remote ~1100 ns (1.5x difference).

4.1.2 Shared Queue Performance

```
[6]: def parse_shared_results(filepath):
         with open(filepath, 'r') as f: content = f.read()
         h2d = re.findall(r'Running host_to_device_memcpy_ce\.\nmemcpy CE CPU\(row\)␣
      ↪-> GPU\(column\) bandwidth \(GB/s\)\n\s+0\n\s*0\s+([\d\.]+)', content)
         numa = re.findall(r'cpubind: (\d+)\s*\n', content)
         return {'h2d_bandwidth': [float(x) for x in h2d], 'numa_nodes': [int(x) for␣
      ↪x in numa]}

     shared_1gpu_data = []
     for i in range(4):
         filepath = RESULTS_DIR / f'shared_array_1gpu_node{i}.txt'
         if filepath.exists():
             data = parse_shared_results(filepath)
             if data['h2d_bandwidth']:
                 shared_1gpu_data.append({'job': i, 'numa': data['numa_nodes'][0] if␣
      ↪data['numa_nodes'] else None, 'h2d': data['h2d_bandwidth'][0]})
     shared_1gpu_df = pd.DataFrame(shared_1gpu_data)
```

```
[7]: fig, ax = plt.subplots(figsize=(10, 6))
categories = ['Exclusive\n(Local GPU)', 'Exclusive\n(Remote GPU)', 'Shared\n(1␣
  ↪GPU/job)']
values = [np.mean(local_h2d), np.mean(remote_h2d), shared_1gpu_df['h2d'].mean()␣
  ↪if len(shared_1gpu_df) > 0 else 0]
errors = [np.std(local_h2d), np.std(remote_h2d), shared_1gpu_df['h2d'].std() if␣
  ↪len(shared_1gpu_df) > 0 else 0]
bars = ax.bar(categories, values, yerr=errors, capsize=5, color=['#2ecc71',␣
  ↪'#e74c3c', '#3498db'], edgecolor='black')
ax.set_ylabel('Bandwidth (GB/s)'); ax.set_title('Host-to-Device Bandwidth␣
  ↪Comparison'); ax.set_ylim(0, 500)
for bar, val in zip(bars, values):
    ax.text(bar.get_x() + bar.get_width()/2, bar.get_height() + 15, f'{val:.
  ↪0f}', ha='center', va='bottom', fontweight='bold')
plt.tight_layout(); plt.savefig('img/bandwidth_comparison.png', dpi=150,␣
  ↪bbox_inches='tight'); plt.show()
```



0.4.2 4.2 Bandwidth Summary

Metric	Local	Remote	Ratio
H2D Bandwidth	411.6 GB/s	88.6 GB/s	4.65x
D2H Bandwidth	169.4 GB/s	88.3 GB/s	1.9x
Latency	739 ns	1109 ns	1.5x

In shared mode, SLURM assigned CPUs from the NUMA package with GPU affinity. Shared queue bandwidth matched exclusive local bandwidth.

0.4.3 4.3 GROMACS Benchmark

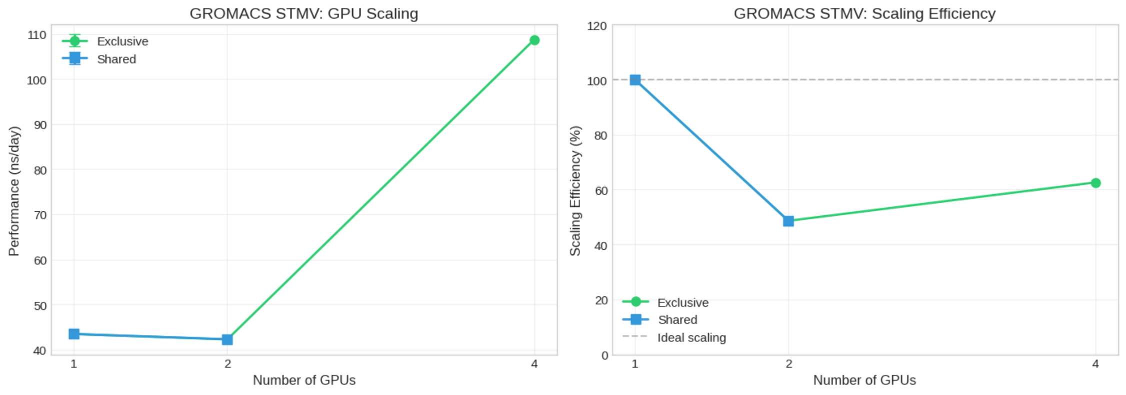
To validate bandwidth findings with a real application, we ran GROMACS molecular dynamics simulations.

Configuration: - System: STMV (~1M atoms) - GROMACS 2023.2 (NVIDIA container) - GPU offloading: nb, bonded, pme - 100,000 steps, performance measured from step 90,000

[8]:
```python
# GROMACS Results Parser - GPU Scaling
GROMACS_LOGS_DIR = Path('../../data/gromacs/logs')

def parse_gromacs_results():
    """Parse all GROMACS output logs."""
    exclusive_results = []
    shared_results = []

    # Parse exclusive queue results
    for filepath in sorted(GROMACS_LOGS_DIR.glob('gromacs_exclusive_*.out')):
        content = filepath.read_text()

        # Find GPU sections and their corresponding performance
        gpu_sections = re.findall(r'Running GROMACS with (\d+) GPU', content)
        performances = re.findall(r'Performance:\s+([\d.]+)\s+[\d.]+', content)

        # Match GPU counts with performance values
        for i, (num_gpus, perf) in enumerate(zip(gpu_sections, performances)):
            exclusive_results.append({
                'num_gpus': int(num_gpus),
                'performance_ns_day': float(perf),
                'queue': 'exclusive'
            })

    # Parse shared queue results
    for filepath in sorted(GROMACS_LOGS_DIR.glob('gromacs_shared_*gpu_*.out')):
        content = filepath.read_text()

        # Extract GPU count from filename
        gpu_match = re.search(r'shared_(\d+)gpu', filepath.name)
        num_gpus = int(gpu_match.group(1)) if gpu_match else None

        # Get performance
        perf_match = re.findall(r'Performance:\s+([\d.]+)\s+[\d.]+', content)
        if perf_match and num_gpus:
            shared_results.append({
                'num_gpus': num_gpus,
                'performance_ns_day': float(perf_match[-1]),
                'queue': 'shared'
            })

    return pd.DataFrame(exclusive_results), pd.DataFrame(shared_results)

gromacs_exclusive_df, gromacs_shared_df = parse_gromacs_results()

print("=== GROMACS GPU Scaling Results ===\n")

if len(gromacs_exclusive_df) > 0:
    print("Exclusive Queue:")
    display(gromacs_exclusive_df)
    print()

if len(gromacs_shared_df) > 0:
    print("Shared Queue:")
    display(gromacs_shared_df)
```

```
=== GROMACS GPU Scaling Results ===

Exclusive Queue:

   num_gpus  performance_ns_day      queue
0         1              43.450  exclusive
1         2              42.246  exclusive
2         4             108.752  exclusive


Shared Queue:

   num_gpus  performance_ns_day   queue
0         1              43.449  shared
1         2              42.280  shared
```

[9]:
```
# GROMACS GPU Scaling Comparison Plot
all_results = pd.concat([gromacs_exclusive_df, gromacs_shared_df],␣
↪ignore_index=True) if len(gromacs_exclusive_df) > 0 or␣
↪len(gromacs_shared_df) > 0 else pd.DataFrame()

if len(all_results) > 0:
    fig, axes = plt.subplots(1, 2, figsize=(14, 5))

    # Plot 1: Performance by GPU count
    ax1 = axes[0]

    # Group by queue and num_gpus
    for queue, color, marker in [('exclusive', '#2ecc71', 'o'), ('shared',␣
↪'#3498db', 's')]:
        df = all_results[all_results['queue'] == queue]
        if len(df) > 0:
            grouped = df.groupby('num_gpus')['performance_ns_day'].agg(['mean',␣
↪'std'])
            ax1.errorbar(grouped.index, grouped['mean'], yerr=grouped['std'],
                         label=f'{queue.capitalize()}', marker=marker, capsize=5,
                         linewidth=2, markersize=8, color=color)

    ax1.set_xlabel('Number of GPUs')
    ax1.set_ylabel('Performance (ns/day)')
    ax1.set_title('GROMACS STMV: GPU Scaling')
    ax1.legend()
    ax1.set_xticks([1, 2, 4])
    ax1.grid(True, alpha=0.3)

    # Plot 2: Scaling efficiency (relative to 1 GPU)
    ax2 = axes[1]

    for queue, color, marker in [('exclusive', '#2ecc71', 'o'), ('shared',␣
↪'#3498db', 's')]:
        df = all_results[all_results['queue'] == queue]
        if len(df) > 0:
            grouped = df.groupby('num_gpus')['performance_ns_day'].mean()
            if 1 in grouped.index:
                baseline = grouped[1]
                efficiency = (grouped / baseline) / grouped.index * 100
                ax2.plot(grouped.index, efficiency, marker=marker,␣
↪label=f'{queue.capitalize()}',
                         linewidth=2, markersize=8, color=color)

    ax2.axhline(y=100, color='gray', linestyle='--', alpha=0.5, label='Ideal␣
↪scaling')
    ax2.set_xlabel('Number of GPUs')
    ax2.set_ylabel('Scaling Efficiency (%)')
    ax2.set_title('GROMACS STMV: Scaling Efficiency')
    ax2.legend()
    ax2.set_xticks([1, 2, 4])
    ax2.set_ylim(0, 120)
    ax2.grid(True, alpha=0.3)

    plt.tight_layout()
    plt.savefig('img/gromacs_scaling.png', dpi=150, bbox_inches='tight')
    plt.show()
else:
    print("No GROMACS results available yet. Run the benchmark scripts:")
    print("  sbatch scripts/gromacs/gromacs_exclusive.slurm")
    print("  sbatch scripts/gromacs/gromacs_shared_1gpu.slurm")
    print("  sbatch scripts/gromacs/gromacs_shared_2gpu.slurm")
```



GROMACS Results

Queue	GPUs	ns/day	Scaling
Exclusive	1	43.45	1.00x
Exclusive	2	42.25	0.97x
Exclusive	4	108.75	2.50x
Shared	1	43.45	1.00x
Shared	2	42.28	0.97x

Observations: - Single-GPU: Identical performance in both queues - 2-GPU: Slight performance decrease versus 1-GPU (communication overhead) - 4-GPU: 2.5x speedup (62.5% efficiency)

[10]:
```
summary_data = {
    'Metric': ['H2D Bandwidth (Local)', 'H2D Bandwidth (Remote)', 'D2H␣
 ↪Bandwidth (Local)',
               'D2H Bandwidth (Remote)', 'Latency (Local)', 'Latency (Remote)',␣
 ↪'Local/Remote BW Ratio'],
    'Value': [f'{np.mean(local_h2d):.1f} GB/s', f'{np.mean(remote_h2d):.1f} GB/
 ↪s',
              f'{np.mean([d2h_df.iloc[i, i] for i in range(4)]):.1f} GB/s',
              f'{np.mean([d2h_df.iloc[i, j] for i in range(4) for j in range(4)␣
 ↪if i != j]):.1f} GB/s',
              f'{np.mean(local_lat):.0f} ns', f'{np.mean(remote_lat):.0f} ns',␣
 ↪f'{np.mean(local_h2d)/np.mean(remote_h2d):.2f}x']
}
pd.DataFrame(summary_data)
```

[10]:
```
                   Metric       Value
0   H2D Bandwidth (Local)  411.6 GB/s
1  H2D Bandwidth (Remote)   88.6 GB/s
```

```
2   D2H Bandwidth (Local)  169.4 GB/s
3  D2H Bandwidth (Remote)   88.3 GB/s
4         Latency (Local)     739 ns
5        Latency (Remote)    1109 ns
6   Local/Remote BW Ratio      4.65x
```

0.5 5. Conclusions

Bandwidth: - Local GPU access: 411 GB/s H2D, 169 GB/s D2H - Remote GPU access: 88 GB/s (4.6x slower) - Shared queue maintained NUMA locality

GROMACS (STMV): - Single-GPU: 43.45 ns/day in both queues - 2-GPU: No scaling benefit - 4-GPU: 2.5x speedup

Practical guidance: - Single-GPU jobs: Shared queue has no performance penalty - Multi-GPU GROMACS (STMV): Use 1 or 4 GPUs

---

0.6 6. References

1. NVIDIA GH200 Grace Hopper Superchip Documentation - https://www.nvidia.com/en-us/data-center/grace-hopper-superchip/
2. SLURM Generic Resource (GRES) Scheduling - https://slurm.schedmd.com/gres.html
3. SDumont II User Manual - https://github.com/lncc-sered/manual-sdumont2nd
4. NVIDIA nvbandwidth Tool - https://github.com/NVIDIA/nvbandwidth
5. NVIDIA GH200 Benchmark Guide - https://docs.nvidia.com/gh200-superchip-benchmark-guide.pdf

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0.7 Appendix: Scripts and Data

Bandwidth scripts (`scripts/transfer/`): `exclusive.slurm`, `shared_array_1gpu.slurm`, `shared_array_2gpu.slurm`

GROMACS scripts (`scripts/gromacs/`): `gromacs_exclusive.slurm`, `gromacs_shared_1gpu.slurm`, `gromacs_shared_2gpu.slurm`

Data (`data/`): Raw benchmark outputs in `transfer/` and `gromacs/logs/`