

Agenda

- Introduction
- **Roofline Fundamentals**
- Empirical Hierarchical Roofline on MI200
 - **Roofline Overview**
 - **Roofline Arithmetic**
 - **Empirical Roofline Benchmarking**
- **Roofline Analysis Workflow**
 - **Tooling**
 - **Features**
 - **Bottleneck Analysis Recipe**
- Examples
 - Add/Mul/FMA
 - N-Body
- **HPC Application Results**



AMD Fueling the Era of Exascale

OAK RIDGE FRONTIER





LAWRENCE LIVERMORE EL CAPITAN



AMD INSTINCT™ MI250X ACCELERATOR

TSMC 6NM **TECHNOLOGY**

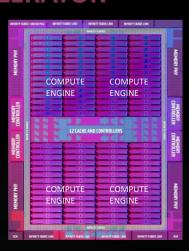
4 MATRIX CORES PER COMPUTE UNIT

8 INFINITY FABRIC LINKS PER DIE

UP TO 110 CU PER **GRAPHICS COMPUTE DIE**

MATRIX CORES ENHANCED FOR HPC

SPECIAL FP32 OPS FOR **DOUBLE THROUGHPUT**

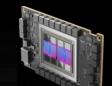


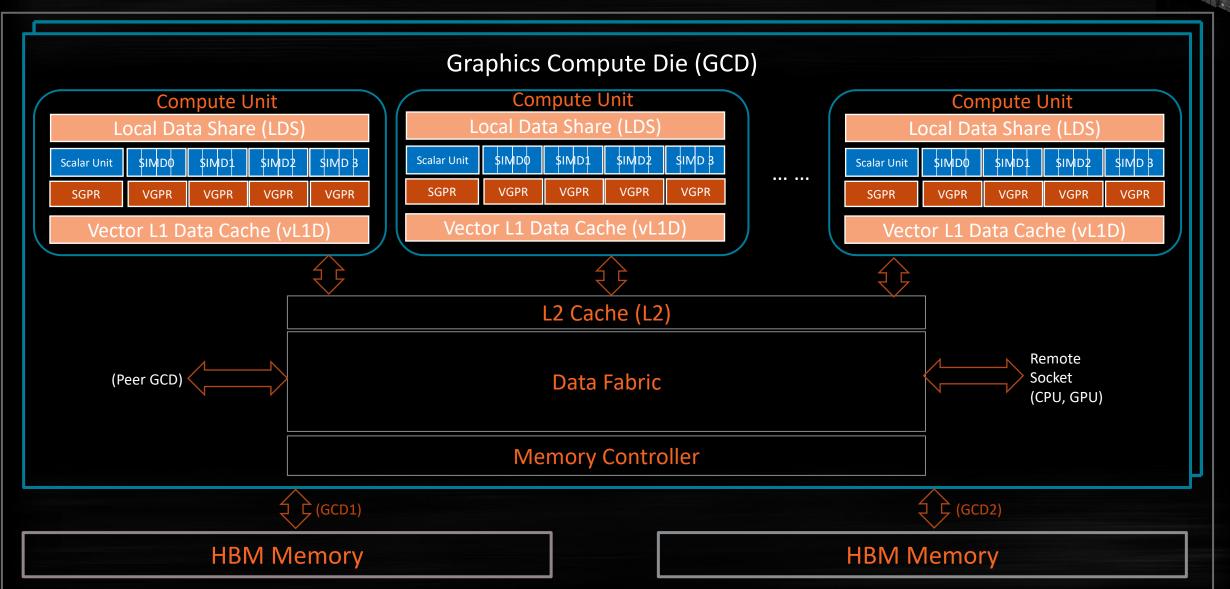
FRONTIER NODE AT A GLANCE

- Optimized 3rd Gen AMD EPYC[™] processor
- Four Instinct MI250X accelerators
- Coherent connectivity
 - Via Infinity Fabric™ interconnect
 - Tightly integrated
 - Unified memory space



Overview - AMD Instinct™ MI200 Architecture





Roofline – All Workloads







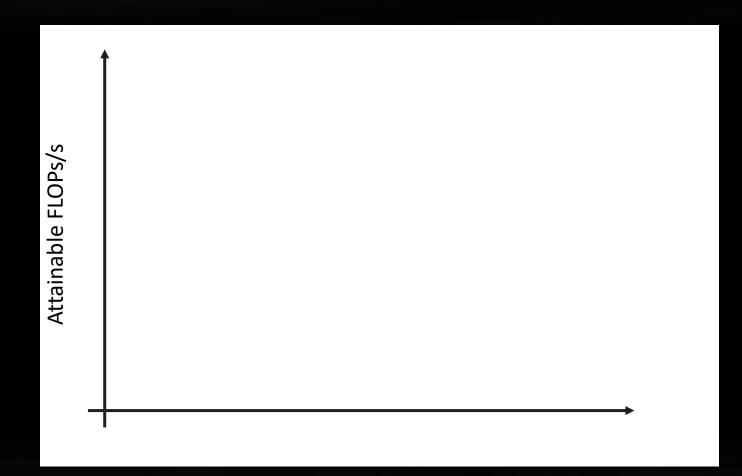
- Attainable FLOPs/s
 - FLOPs/s rate as measured empirically on a given device
 - FLOP = floating point operation
 - FLOP counts for common operations

Add: 1 FLOP

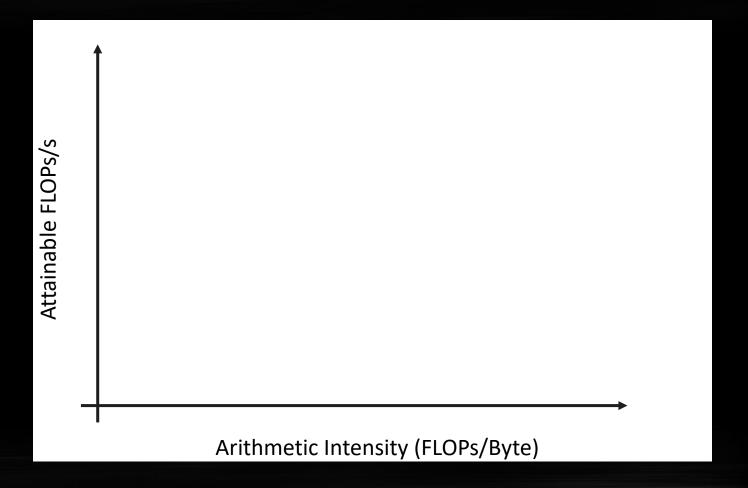
Mul: 1 FLOP

FMA: 2 FLOP

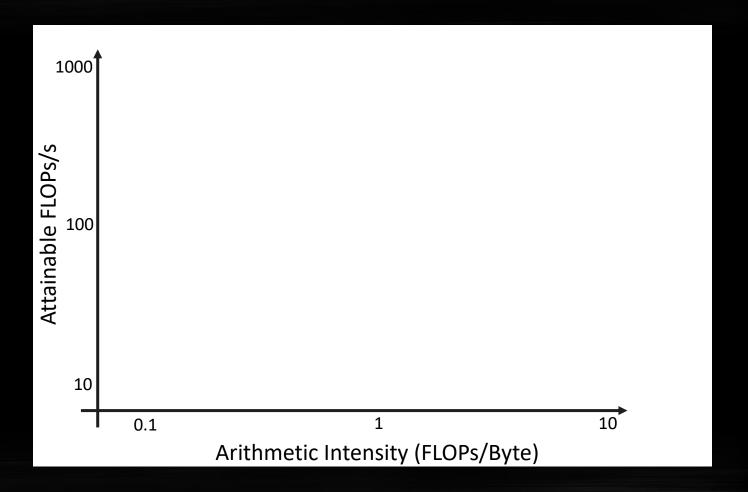
FLOPs/s = Number of floating-point operations performed per second



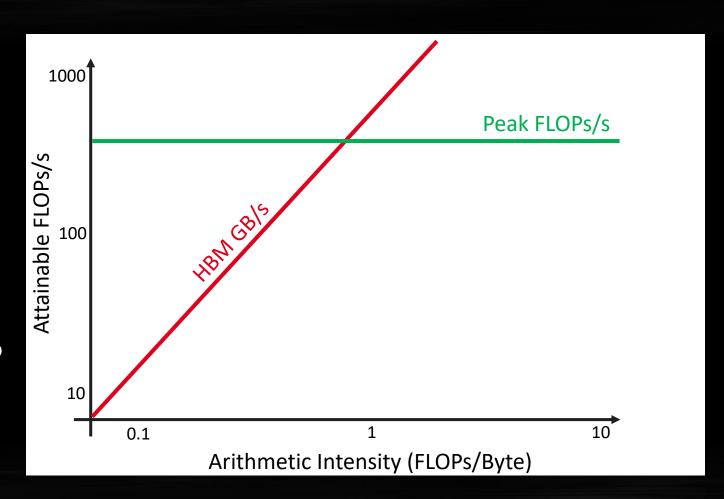
- Arithmetic Intensity (AI)
 - characteristic of the workload indicating how much compute (FLOPs) is performed per unit of data movement (Byte)
 - Ex: x[i] = y[i] + c
 - FLOPs = 1
 - Bytes = 1xRD + 1xWR = 4 + 4 = 8
 - AI = 1/8



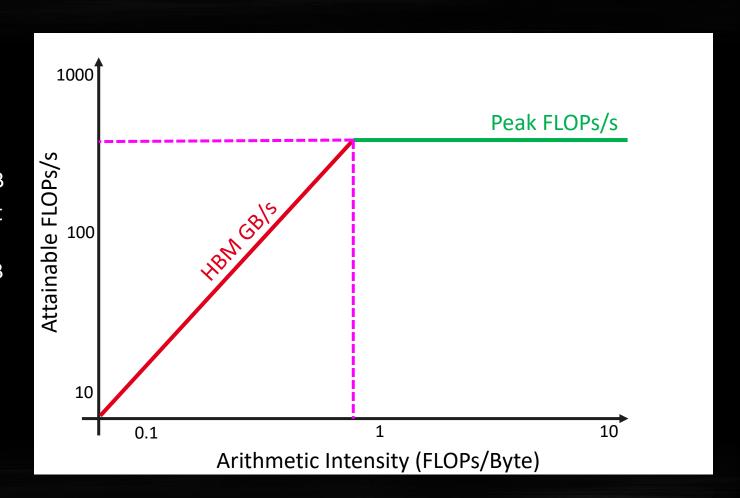
- Log-Log plot
 - makes it easy to doodle, extrapolate performance along Moore's Law, etc...



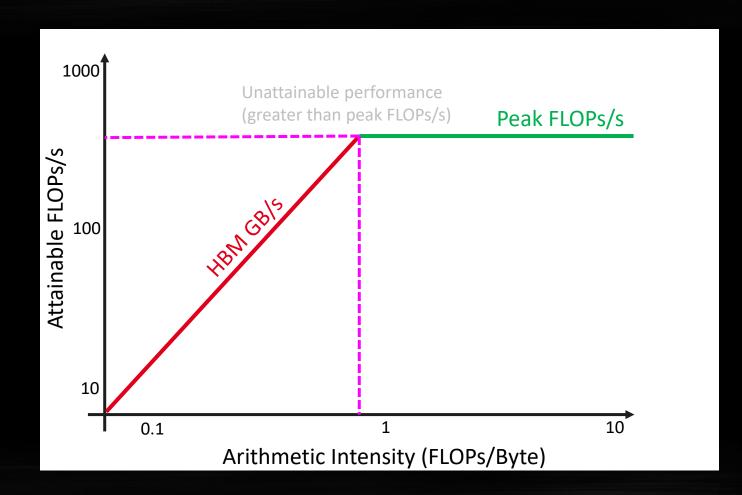
- **Roofline Limiters**
 - Compute
 - Peak FLOPs/s
 - Memory BW
 - Al * Peak GB/s
- Note:
 - These are empirically measured values
 - Different SKUs will have unique plots
 - Individual devices within a SKU will have slightly different plots based on thermal solution, system power, etc.
 - MIBench uses suite of simple kernels to empirically derive these values
 - These are **NOT** theoretical values indicating peak performance under "unicorn" conditions



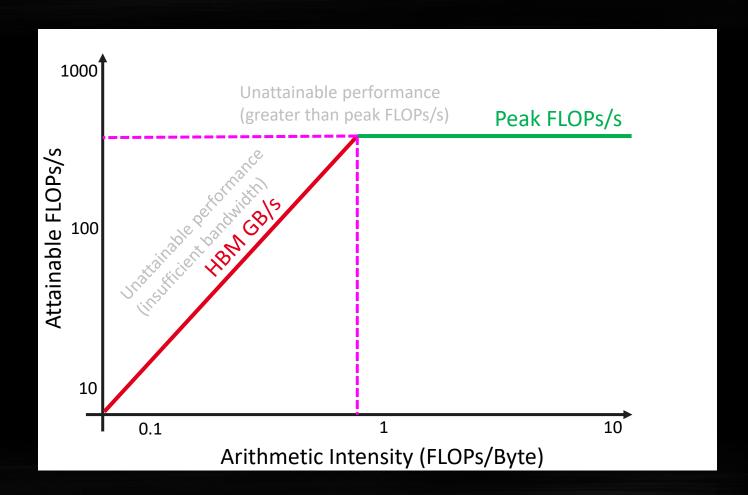
- Attainable FLOPs/s =
- Machine Balance:
 - Where $AI = \frac{Peak\ FLOPs/s}{Peak\ GB/s}$
 - Typical machine balance: 5-10 FLOPs/B
 - **40-80** FLOPs per double to exploit compute capability
 - MI250x machine balance: ~16 FLOPs/B
 - **128** FLOPs per double to exploit compute capability



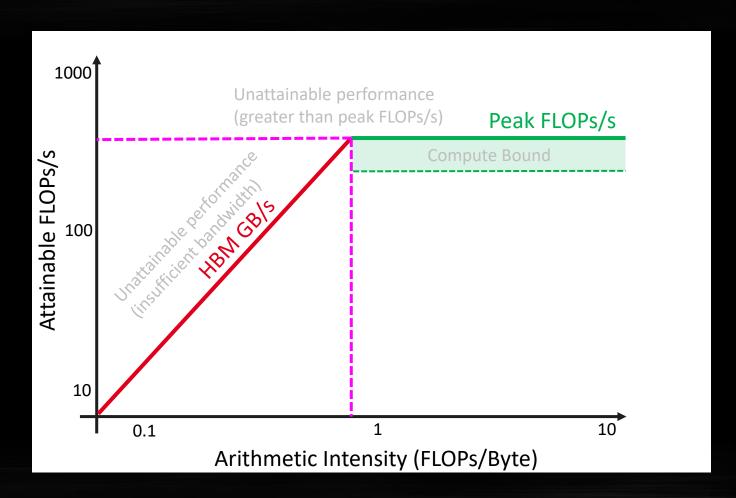
- Attainable FLOPs/s =
- Machine Balance:
 - Where $AI = \frac{Peak \ FLOPs/s}{Peak \ GB/s}$
- Five Performance Regions:
 - **Unattainable Compute**



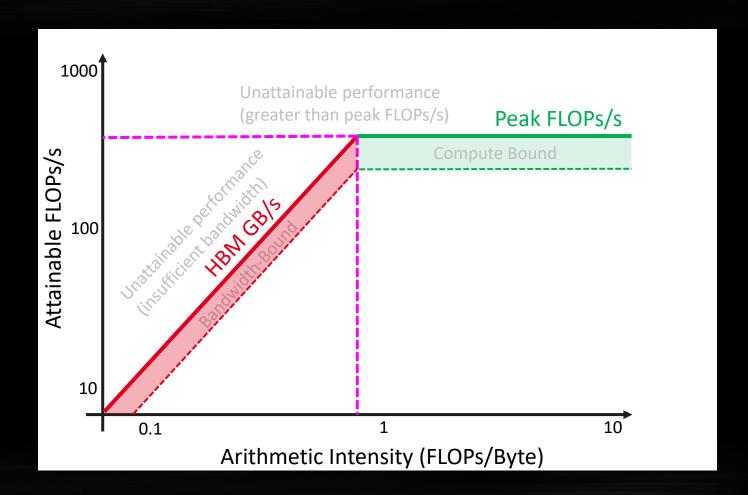
- Attainable FLOPs/s =
 - $min \begin{cases} Peak FLOPs/s \\ AI * Peak GB/s \end{cases}$
- Machine Balance:
 - Where $AI = \frac{Peak \ FLOPs/s}{Peak \ GB/s}$
- Five Performance Regions:
 - **Unattainable Compute**
 - Unattainable Bandwidth



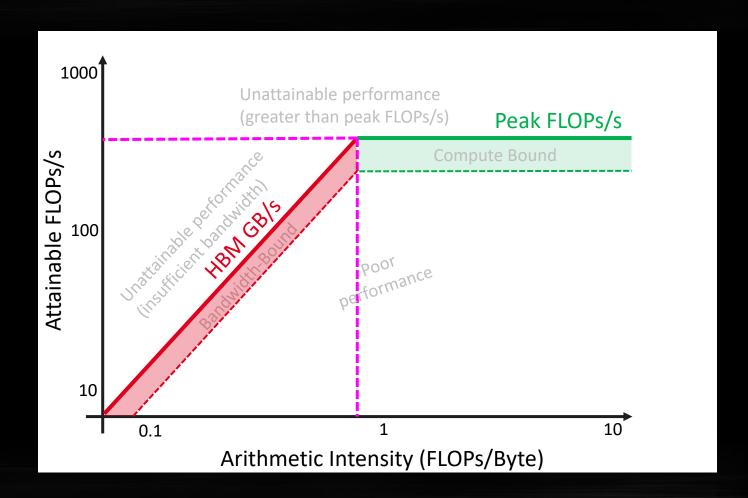
- Attainable FLOPs/s =
- Machine Balance:
 - Where $AI = \frac{Peak \ FLOPs/s}{Peak \ GB/s}$
- Five Performance Regions:
 - **Unattainable Compute**
 - Unattainable Bandwidth
 - Compute Bound



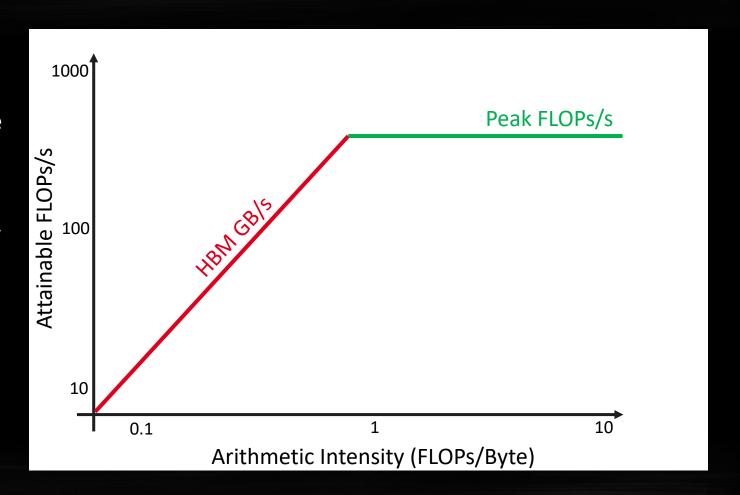
- Attainable FLOPs/s =
- Machine Balance:
 - Where $AI = \frac{Peak FLOPs/s}{Peak GB/s}$
- Five Performance Regions:
 - **Unattainable Compute**
 - Unattainable Bandwidth
 - Compute Bound
 - Bandwidth Bound



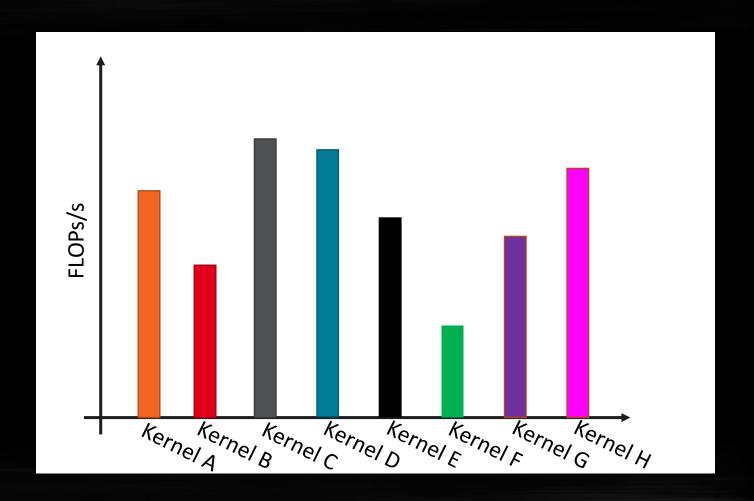
- Attainable FLOPs/s =
- Machine Balance:
 - Where $AI = \frac{Peak FLOPs/s}{Peak GB/s}$
- Five Performance Regions:
 - **Unattainable Compute**
 - Unattainable Bandwidth
 - Compute Bound
 - Bandwidth Bound
 - Poor Performance



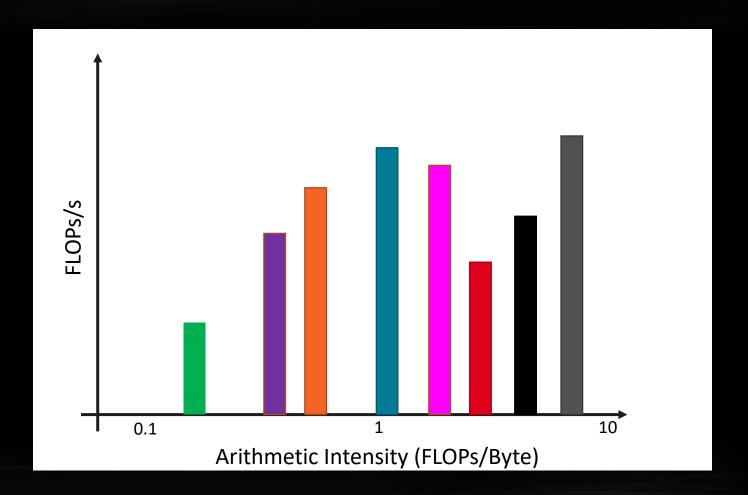
- Attainable FLOPs/s =
- Final result is a single roofline plot presenting the peak attainable performance (in terms of FLOPs/s) on a given device based on the arithmetic intensity of any potential workload
- We have an application independent way of measuring and comparing performance on any platform



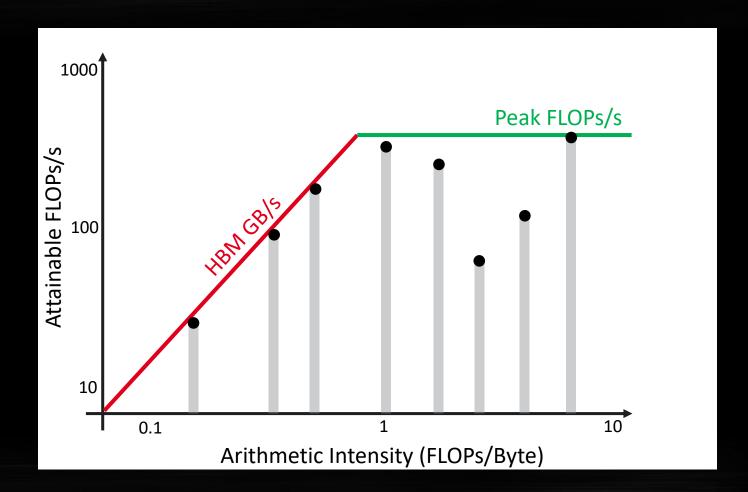
- Example:
 - We run a number of kernels and measure FLOPs/s



- Example:
 - We run a number of kernels and measure FLOPs/s
 - Sort kernels by arithmetic intensity

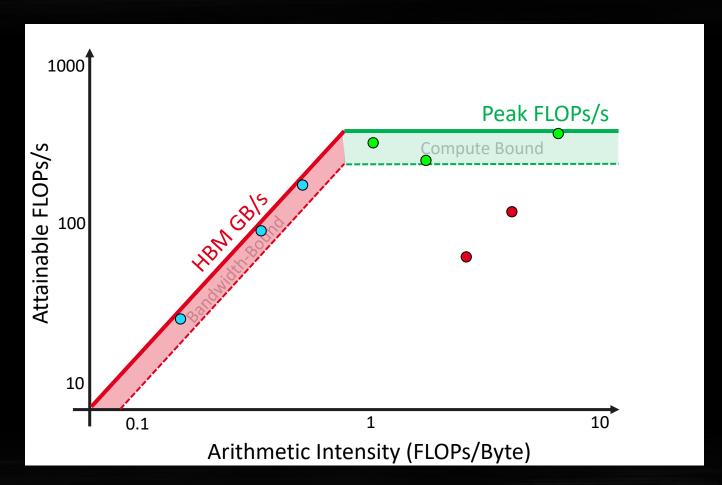


- Example:
 - We run a number of kernels and measure FLOPs/s
 - Sort kernels by arithmetic intensity
 - Compare performance relative to hardware capabilities



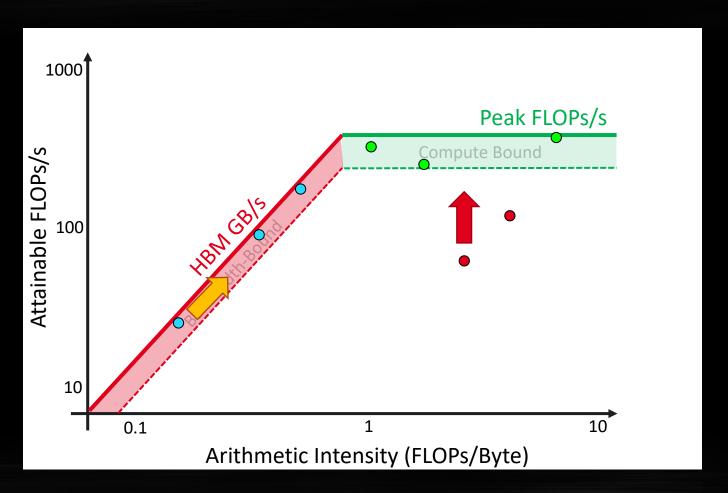
Example:

- We run a number of kernels and measure FLOPs/s
- Sort kernels by arithmetic intensity
- Compare performance relative to hardware capabilities
- Kernels near the roofline are making good use of computational resources
 - Kernels can have low performance (FLOPS/s), but make good use of BW

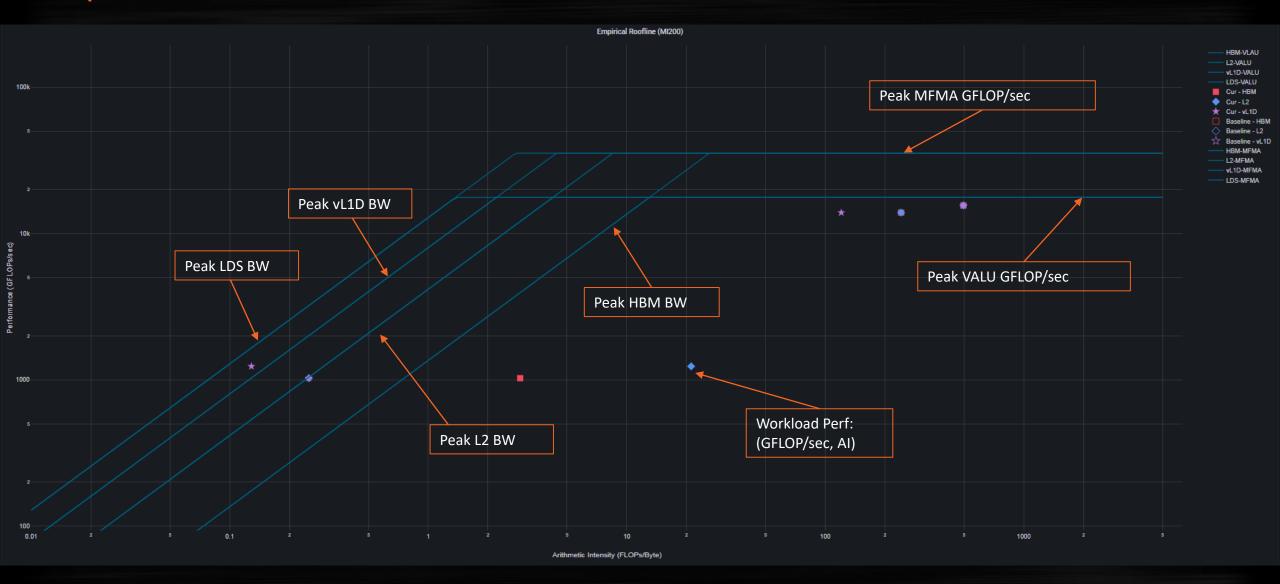


Example:

- We run a number of kernels and measure FLOPs/s
- Sort kernels by arithmetic intensity
- Compare performance relative to hardware capabilities
- Kernels near the roofline are making good use of computational resources
 - Kernels can have low performance (FLOPS/s), but make good use of BW
- Increase arithmetic intensity when bandwidth limited
 - Reducing data movement increases Al
- Kernels not near the roofline should* have optimizations that can be made to get closer to the roofline



Empirical Hierarchical Roofline on MI200 - Overview



Empirical Roofline Benchmarking (MIPerf)

- Empirical Roofline Benchmarking
 - Measure achievable Peak FLOPS
 - VALU: F32, F64
 - MFMA: F16, BF16, F32, F64
 - Measure achievable Peak BW
 - LDS
 - Vector L1D Cache
 - L2 Cache
 - HBM
- Internally developed micro benchmark algorithms
 - Peak VALU FLOP: axpy
 - Peak MFMA FLOP: Matrix multiplication based on MFMA intrinsic
 - Peak LDS/vL1D/L2 BW: Pointer chasing
 - Peak HBM BW: Streaming copy

```
amd@node-bp126-014a utils ±|master x|→ ./roofline
Total detected GPU devices: 2
GPU Device 0: Profiling...
GPU ID: 0, workgroupSize:256, workgroups:8192, experiments:100, Total Bytes=687194767360, Duration=157.3 ms, Mean=4321.3 GB/sec, stdev=59.1 GB/s
   GPU ID: 0, workgroupSize:256, workgroups:16384, experiments:100, Total Bytes=26843545600, Duration=3.3 ms, Mean=8262.6 GB/sec, stdev=5.9 GB/s
```

Roofline Arithmetic: Perfmon Counters

Weight

- ADD: 1

- MUL: 1

- FMA: 2

- Transcendental: 1

FLOP Count

VALU: derived from VALU math instructions (assuming 64 active threads)

• MFMA: count FLOP directly, in unit of 512

Transcendental Instructions (7 in total)

• e^x , $\log(x)$: F16, F32

 $-\frac{1}{x}$, \sqrt{x} , $\frac{1}{\sqrt{x}}$: F16, F32, F64

- $\sin x$, $\cos x$: F16, F32

Profiling Overhead

Require 3 application replays

v_rcp_f64_e32 v[4:5], v[2:3] v_sin_f32_e32 v2, v2 v_cos_f32_e32 v2, v2 v_rsq_f64_e32 v[6:7], v[2:3] v_sqrt_f32_e32 v3, v2 v_log_f32_e32 v2, v2 v_exp_f32_e32 v2, v2

ID	HW Counter	Category
1	SQ_INSTS_VALU_ADD_F16	FLOP counter
2	SQ_INSTS_VALU_MUL_F16	FLOP counter
3	SQ_INSTS_VALU_FMA_F16	FLOP counter
4	SQ_INSTS_VALU_TRANS_F16	FLOP counter
5	SQ_INSTS_VALU_ADD_F32	FLOP counter
6	SQ_INSTS_VALU_MUL_F32	FLOP counter
7	SQ_INSTS_VALU_FMA_F32	FLOP counter
8	SQ_INSTS_VALU_TRANS_F32	FLOP counter
9	SQ_INSTS_VALU_ADD_F64	FLOP counter
10	SQ_INSTS_VALU_MUL_F64	FLOP counter
11	SQ_INSTS_VALU_FMA_F64	FLOP counter
12	SQ_INSTS_VALU_TRANS_F64	FLOP counter
13	SQ_INSTS_VALU_INT32	IOP counter
14	SQ_INSTS_VALU_INT64	IOP counter
15	SQ_INSTS_VALU_MFMA_MOPS_I8	IOP counter

ID	HW Counter	Category
16	SQ_INSTS_VALU_MFMA_MOPS_F16	FLOP counter
17	SQ_INSTS_VALU_MFMA_MOPS_BF16	FLOP counter
18	SQ_INSTS_VALU_MFMA_MOPS_F32	FLOP counter
19	SQ_INSTS_VALU_MFMA_MOPS_F64	FLOP counter
20	SQ_LDS_IDX_ACTIVE	LDS Bandwidth
21	SQ_LDS_BANK_CONFLICT	LDS Bandwidth
22	TCP_TOTAL_CACHE_ACCESSES_sum	vL1D Bandwidth
23	TCP_TCC_WRITE_REQ_sum	L2 Bandwidth
24	TCP_TCC_ATOMIC_WITH_RET_REQ_sum	L2 Bandwidth
25	TCP_TCC_ATOMIC_WITHOUT_RET_REQ_sum	L2 Bandwidth
26	TCP_TCC_READ_REQ_sum	L2 Bandwidth
27	TCC_EA_RDREQ_sum	HBM Bandwidth
28	TCC_EA_RDREQ_32B_sum	HBM Bandwidth
29	TCC_EA_WRREQ_sum	HBM Bandwidth
30	TCC_EA_WRREQ_64B_sum	HBM Bandwidth

Roofline Arithmetic: Metrics

```
Total_FLOP = 64 * (SQ INSTS VALU ADD F16 + SQ INSTS VALU MUL F16 + SQ INSTS VALU TRANS F16 + 2 * SQ INSTS VALU FMA F16)
            + 64 * (SQ INSTS VALU ADD F32 + SQ INSTS VALU MUL F32 + SQ INSTS VALU TRANS F32 + 2 * SQ INSTS VALU FMA F32)
            + 64 * (SQ INSTS VALU ADD F64 + SQ INSTS VALU MUL F64 + SQ INSTS VALU TRANS F64 + 2 * SQ INSTS VALU FMA F64)
            + 512 * SQ INSTS VALU MFMA MOPS F16
            + 512 * SQ INSTS VALU MFMA MOPS BF16
            + 512 * SQ INSTS VALU MFMA MOPS F32
            + 512 * SQ INSTS VALU MFMA MOPS F64
```

Total_IOP = 64 * (SQ INSTS VALU INT32 + SQ INSTS VALU INT64)

 $LDS_{BW} = 32 * 4 * (SQ LDS IDX ACTIVE - SQ LDS BANK CONFLICT)$

 $vL1D_{BW} = 64 * TCP TOTAL CACHE ACCESSES sum$

$$L2_{BW} = 64 * TCP_TCC_READ_REQ_sum + 64 * TCP_TCC_WRITE_REQ_sum + 64 * (TCP_TCC_ATOMIC_WITH_RET_REQ_sum + TCP_TCC_ATOMIC_WITHOUT_RET_REQ_sum)$$

HBM_{BW} = 32 * TCC_EA_RDREQ_32B_sum + 64 * (TCC_EA_RDREQ_sum - TCC_EA_RDREQ_32B_sum) + 32 * (TCC EA WRREQ sum - TCC EA WRREQ 64B sum) + 64 * TCC EA WRREQ 64B sum



$$AI_{vL1D} \frac{TOTAL_FLOP}{vL1D_{BW}}$$

$$AI_{L2} \frac{TOTAL_FLOP}{L2_{BW}}$$

$$AI_{HBM} = rac{TOTAL_FLOP}{HBM_{BW}}$$



TOTAL FLOP LDSRW

^{*} All calculations are subject to change

Roofline Analysis: Manual Rocprof

- For those who like getting their hands dirty
- Generate input file
 - See example roof-counters.txt →
- Run rocprof

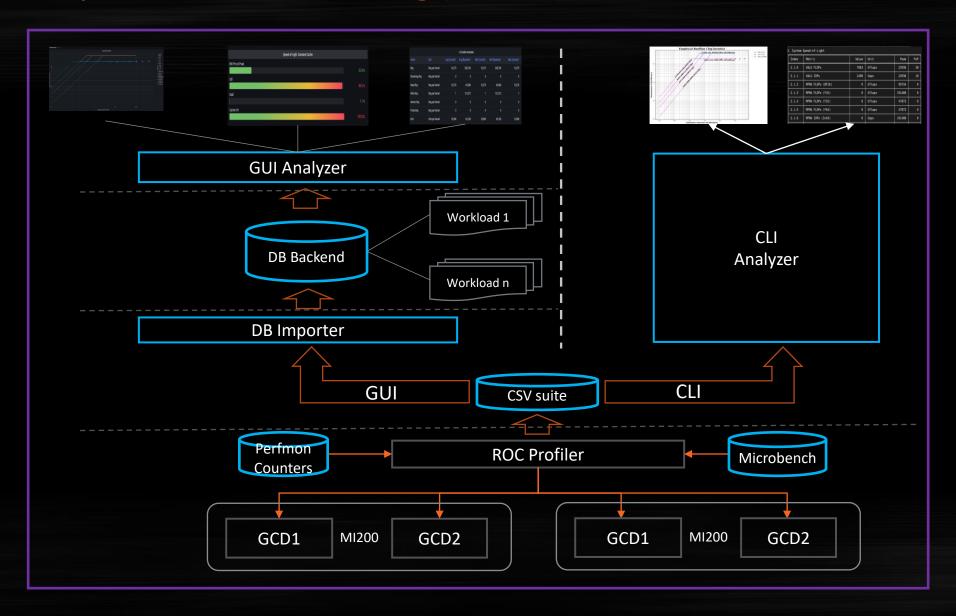
```
foo@bar:~$ rocprof -i roof-counters.txt --timestamp on ./myCoolApp
```

- Analyze results
 - Load results.csv output file in csv viewer of choice
 - Derive final metric values using equations on previous slide
- Profiling Overhead
 - Requires one application replay for each pmc line

```
## roof-counters.txt
# FP32 FLOPs
pmc: SQ_INSTS_VALU_ADD_F32 SQ_INSTS_VALU_MUL_F32 SQ_INSTS_VALU_FMA_F32 SQ_INSTS_VALU_TRANS_F32
# HBM Bandwidth
pmc: TCC_EA_RDREQ_sum TCC_EA_RDREQ_32B_sum TCC_EA_WRREQ_sum TCC_EA_WRREQ_64B_sum
# LDS Bandwidth
pmc: SQ_LDS_IDX_ACTIVE SQ_LDS_BANK_CONFLICT
# L2 Bandwidth
pmc: TCP_TCC_READ_REQ_sum TCP_TCC_WRITE_REQ_sum TCP_TCC_ATOMIC_WITH_RET_REQ_sum
TCP TCC ATOMIC WITHOUT RET REQ sum
# vL1D Bandwidth
pmc: TCP_TOTAL_CACHE_ACCESSES_sum
```



Roofline Analysis Workflow – Tooling (MIPerf)



Roofline Analysis Workflow – Tooling

Workload Profiling

miperf profile -n mixbench-hip -c "./mixbench-hip-ro"

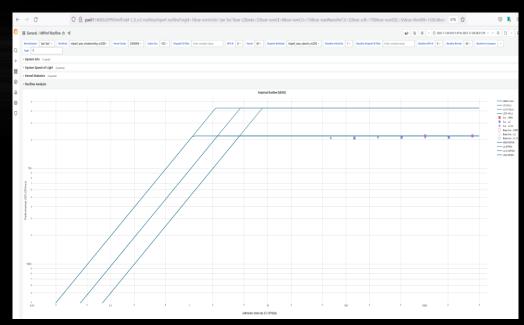
GUI Import

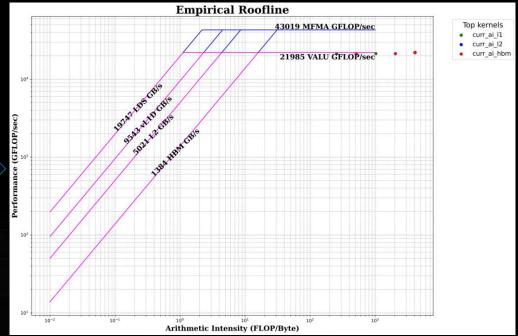
miperf import -i -n mixbenchhip --path workloads/mixbenchhip/mi200/ -H pavii1 -u amd -t asw

CLI Roofline Generation

miperf analyze --gen-roofline -p workloads/mixbench-hip/mi200/ -c "./mixbench-hip-ro"

* All CLI options are subject to change due to fast prototyping. Refer to MI Performance Profiler (MIPerf) -Audacious Software Team - Confluence (amd.com) for the up-to-date documentation.



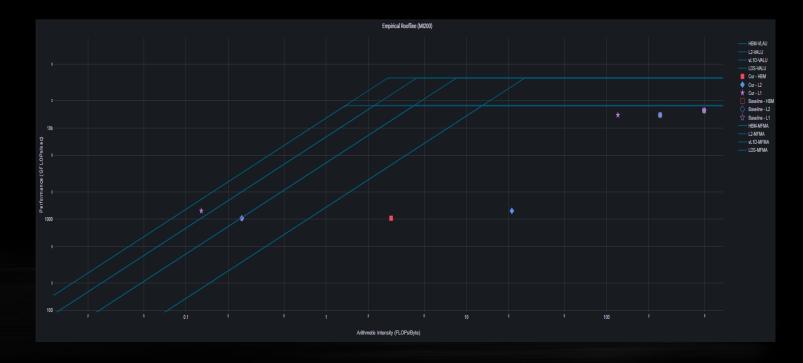




Roofline Analysis Workflow – Features

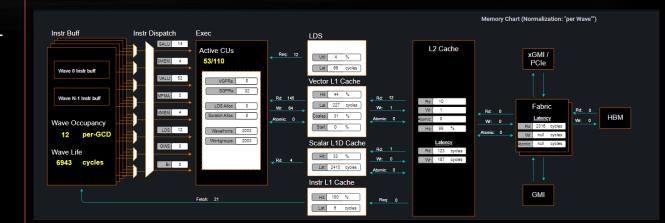
- **GUI** Analyzer
 - Histogram
 - Kernel statistics
 - Kernel filtering
 - Baseline comparison
 - Memory hierarchy selection
- CLI Analyzer
 - Kernel filtering
 - Memory hierarchy selection
 - x/y-axis range selection
 - Pdf/jpg file export





Roofline Analysis Workflow – Bottleneck Analysis Recipes

- Roofline analysis is part of the integrated performance analysis on GPUs
 - Except for simple Compute and Memory BW bound, in-depth profiling and tracing analysis is needed
- Compute Bound workloads
 - Compute Unit Analysis (Instruction Mix, pipeline perf
- Memory BW Bound workloads
 - L2 Cache analysis (BW, Util, cache hit)
 - Vector L1D Cache analysis (BW, Util, cache hit)
 - LDS analysis (BW, Util, latency, bank conflict)
- Memory Latency Bound workloads
 - - Dependency wait, instr issue wait
 - Vector L1D Cache analysis
 - vL1D stall/util/bw/latency
 - Compute Unit analysis
 - VMEM/SMEM/LDS latency
- Dispatch Bound workloads
 - - Waveslot/LDS/VGPR/SGPR limit





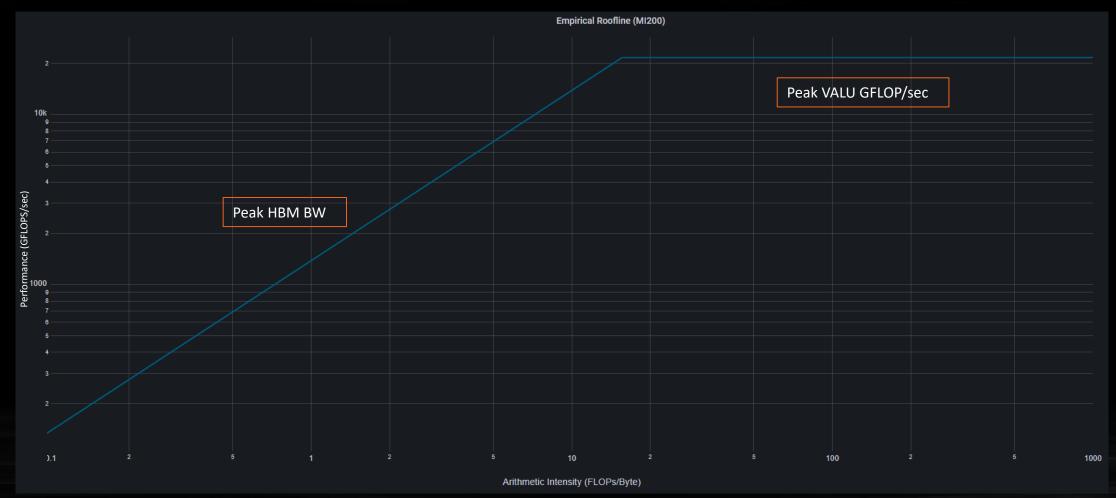
Roofline Examples on AMD Instinct™ MI250X GPU

Roofline Plot – AMD Instinct™ MI250X Accelerators

- Device: Instinct MI250X
 - **ORNL Frontier GPU**

- Instinct MI250X (Dual GCDs)
- Figure shows single GCD

Methodology applies to all AMD Instinct MI200 series GPUs



*AMD Instinct™ MI250X accelerator Datasheet: amd.com/system/files/documents/amd-instinct-mi200-datasheet.pdf



Roofline Example #1 – Add

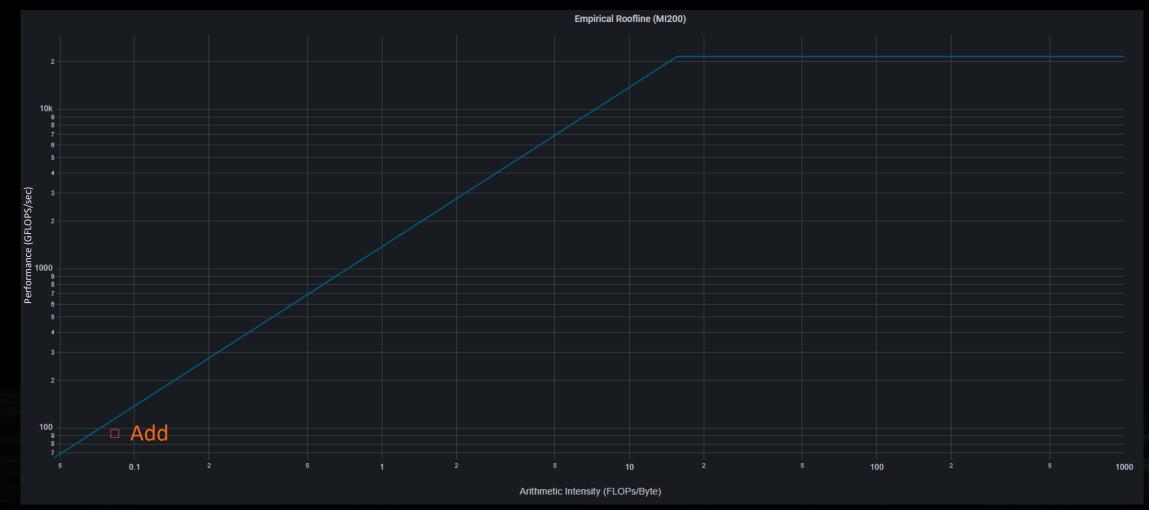
- Calculation:
 - a[i] = a[i] + b[i]
- VALU Ops Per Thread:
 - 1x V ADD
- HBM MEM Ops Per Thread:
 - 2x RD
 - 1x WR
- Arithmetic Intensity:
 - 1 FLOP / (3 * 4Byte) = 1/12

```
1 template<typename T>
 2 __global__ void add_benchmark(T *buf1, T *buf2, uint32_t nSize)
 3 {
 4
       const uint32_t gid = hipBlockDim_x * hipBlockIdx_x + hipThreadIdx_x;
       const uint32 t nThreads = gridDim.x * blockDim.x;
       T *a, *b;
       a = &buf1[gid];
10
       b = &buf2[gid];
11
12
13
       for(uint32_t offset=0; offset < nSize; offset += nThreads)</pre>
14
         a[offset] = a[offset] + b[offset];
15
16
17 }
```

Roofline Example #1 – Add

- Calculation:
 - a[i] = a[i] + b[i]

 Reading two floats for every add results in low arithmetic intensity and HBM limited



Roofline Example #2 – Mul

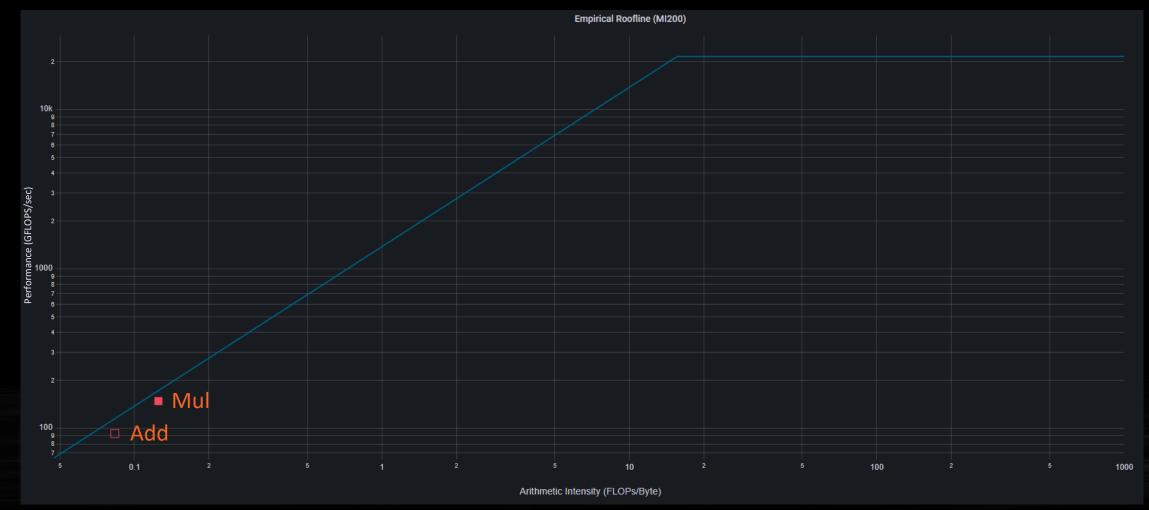
- Calculation:
 - a[i] = x * b[i]
- VALU Ops Per Thread:
 - 1x V MUL
- HBM MEM Ops Per Thread:
 - 1x RD
 - 1x WR
- Arithmetic Intensity:
 - 1 FLOP / (2 * 4Byte) = 1/8

```
1 template<typename T>
 2 __global__ void mul_benchmark(T *buf1, T *buf2, uint32_t nSize)
 3 {
 4
       const uint32_t gid = hipBlockDim_x * hipBlockIdx_x + hipThreadIdx_x;
       const uint32_t nThreads = gridDim.x * blockDim.x;
 5
 6
 7
 8
       T *a, *b;
       a = &buf1[gid];
       b = &buf2[gid];
10
       const T x = (T)1.2;
11
12
13
14
       for(uint32_t offset=0; offset < nSize; offset += nThreads)</pre>
15
         a[offset] = x * b[offset];
16
17
18 }
```

Roofline Example #2 – Mul

- Calculation:
 - a[i] = c * b[i]

Reading one less float (compared to Add) increases our arithmetic intensity and reduces sensitivity to HBM



Roofline Example #3 – Triad

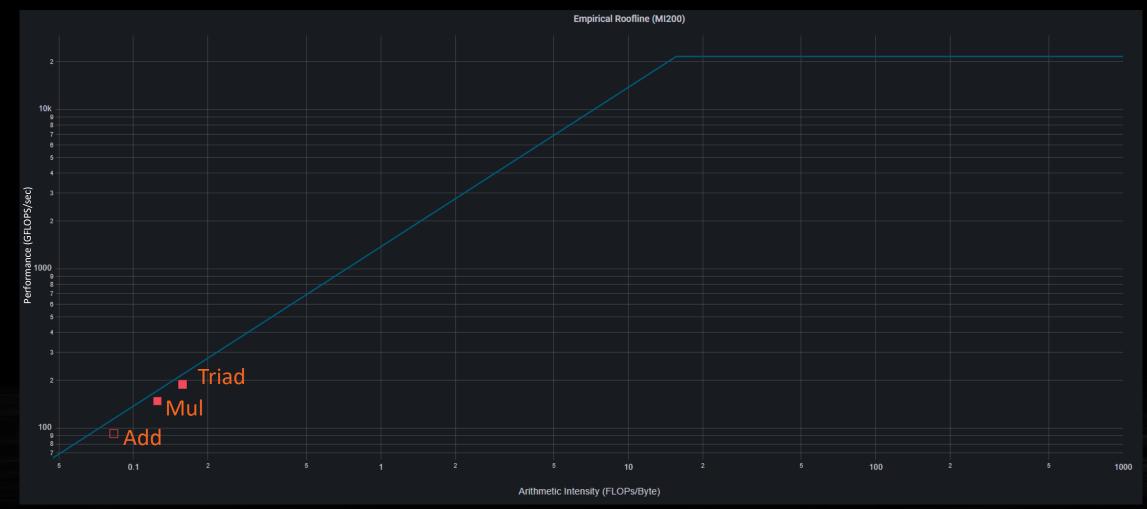
- Calculation:
 - a[i] = b[i] + x * a[i]
- VALU Ops Per Thread:
 - 1x V ADD 1x V_FMA - 1x V MUL
- HBM MEM Ops Per Thread:
 - 2x RD
 - 1x WR
- Arithmetic Intensity:
 - 2 FLOP / (3 * 4Byte) = 1/6

```
1 template<typename T>
 2 _ global _ void triad_benchmark(T *buf1, T *buf2, uint32_t nSize)
 3 {
       const uint32_t gid = hipBlockDim_x * hipBlockIdx_x + hipThreadIdx_x;
       const uint32 t nThreads = gridDim.x * blockDim.x;
       T *a, *b;
       a = &buf1[gid];
       b = &buf2[gid];
10
       const T x = (T)1.2;
11
12
13
       for(uint32_t offset=0; offset < nSize; offset += nThreads)</pre>
14
15
         a[offset] = b[offset] + x * a[offset];
16
17
18 }
```

Roofline Example #3 – Triad

- Calculation:
 - a[i] = b[i] + x * a[i]

 Performing an extra operation increases arithmetic intensity and further reduces sensitivity to HBM as compared to Add and Mul



Roofline Example #4 – FMA

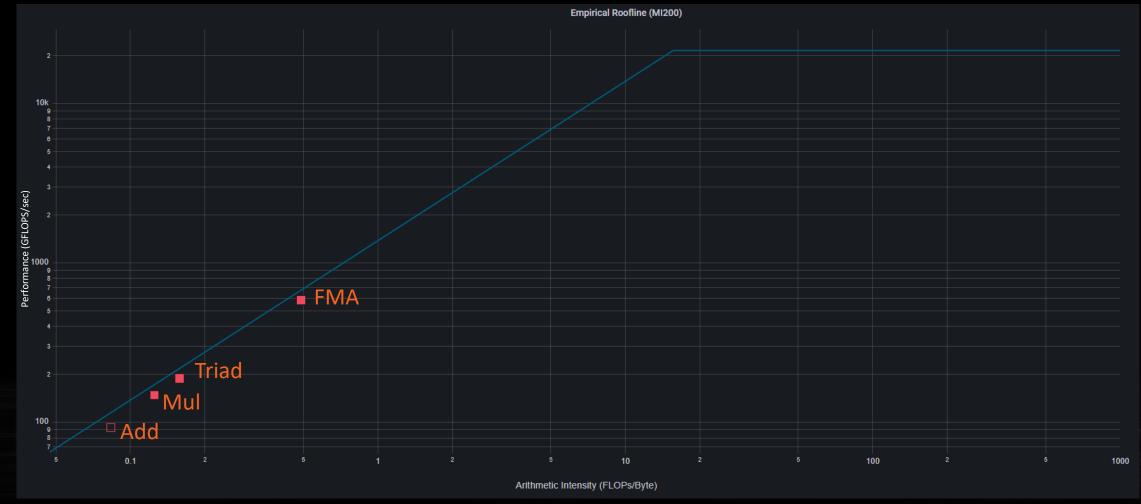
- Calculation:
 - x = a[i] * x + y
- VALU Ops Per Thread:
 - 1x V ADD 1x V_FMA - 1x V MUL
- HBM MEM Ops Per Thread:
 - 1x RD
- Arithmetic Intensity:
 - 2 FLOP / (1 * 4Byte) = 1/2

```
1 template<typename t>
 2 __global__ void flops_benchmark(T *buf, uint32_t nSize)
 3 {
       const uint32_t gid = hipBlockDim_x * hipBlockIdx_x + hipThreadIdx_x;
 4
       const uint32 t nThreads = gridDim.x * blockDim.x;
       T *a;
       a = &buf[gid];
       const T y = (T) 1.0;
       T x = (T) 2.0;
11
12
13
       for(uint32_t offset=0; offset < nSize; offset += nThreads)</pre>
14
15
           x = a[offset] * x + y;
16
17
       a[0] = -x;
19 }
```

Roofline Example #4 – FMA

- Calculation:
 - x = a[i] * x + y

■ Each thread having to load one less value from HBM further increases arithmetic intensity and improves FLOPs/s performance



Roofline Example #5 – FMA 1024

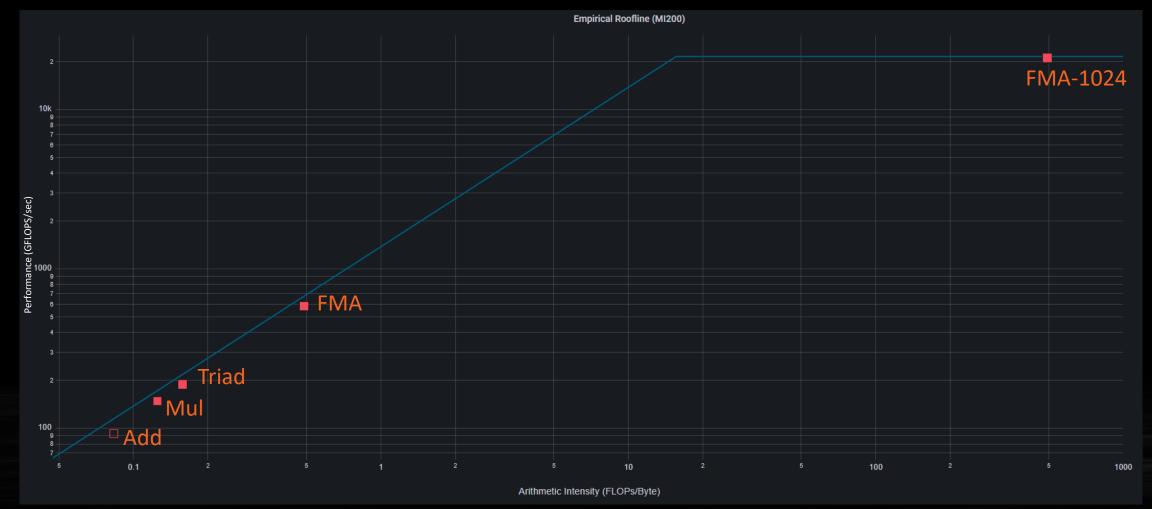
- Calculation:
 - x = a[i] * x + y
- VALU Ops Per Thread:
 - 1x V ADD 1x V_FMA - 1x V MUL
- HBM MEM Ops Per Thread:
 - 1x RD
- Arithmetic Intensity:
 - 1024 * 2 FLOP / (1 * 4Byte) = 512

```
1024
1 template<typename T, int nFMA>
2 global void flops_benchmark(T *buf, uint32_t nSize)
 3 {
       const uint32_t gid = hipBlockDim_x * hipBlockIdx_x + hipThreadIdx_x;
       const uint32 t nThreads = gridDim.x * blockDim.x;
       T *a;
       a = &buf[gid];
       const T y = (T) 1.0;
10
       T x = (T) 2.0;
11
12
13
14
       for(uint32_t offset=0; offset < nSize; offset += nThreads)</pre>
15
           for(int j=0; j<nFMA; j++)</pre>
16
17
               x = [a[offset]] * |x| + |y|
18
19
20
21
       a[0] = -x;
22 }
```

Roofline Example #5 – FMA 1024

- Calculation:
 - x = a[i] * x + y

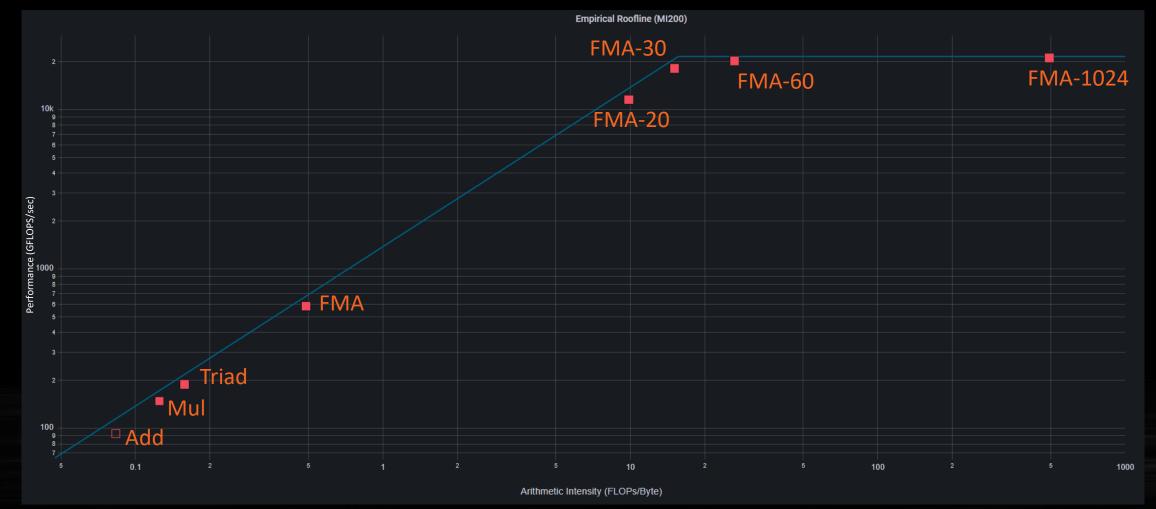
Each thread looping over many FMAs with only one read significantly increases arithmetic intensity and becomes compute VALU limited



Roofline Example #6 – FMA Sweep

- Calculation:
 - x = a[i] * x + y

 Further sweeping the number of FMA instructions from 20 to 60 shows the workload transitioning from HBM limited to VALU limited



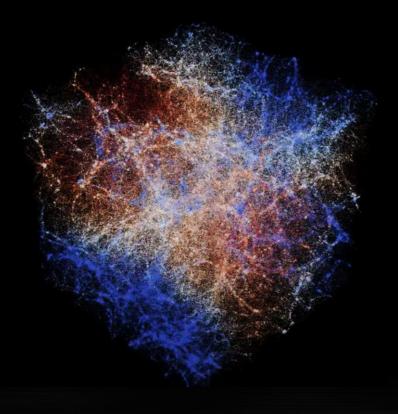
Roofline Use Case - HPC Particle Codes

- Particle interactions form the foundation of many computational science codes from multiple domains
 - <u>Domains</u>: Cosmology, astrophysics, molecular dynamics, and more
 - Applications: HACC, LAMMPS, NAMD, Amber, GROMACS

Nbody

- One such computational algorithm for computing particle interactions leveraged by these applications
- Direct particle-particle method
- Highly accurate
- Computationally expensive (N^2)

HACC – Cosmology



- Repo: https://github.com/ROCm-Developer-Tools/HIP-Examples/tree/master/mini-nbody/hip
 - Fundamental particle-particle algorithm
 - Single collection of N particles calculating N^2 pair-wise interactions
 - Double precision (FP64)
 - Multiple implementations leveraging different optimization approaches
- "orig"
 - Numerical Computing 101 unoptimized implementation
- "soa"
 - Converting particle data layout from array of structures to structure of arrays
- "block"
 - Loading and computing particle data in "tiles" to increase cache hits
- "unroll"
 - Adding #pragma unroll to particle "tile" processing for loop



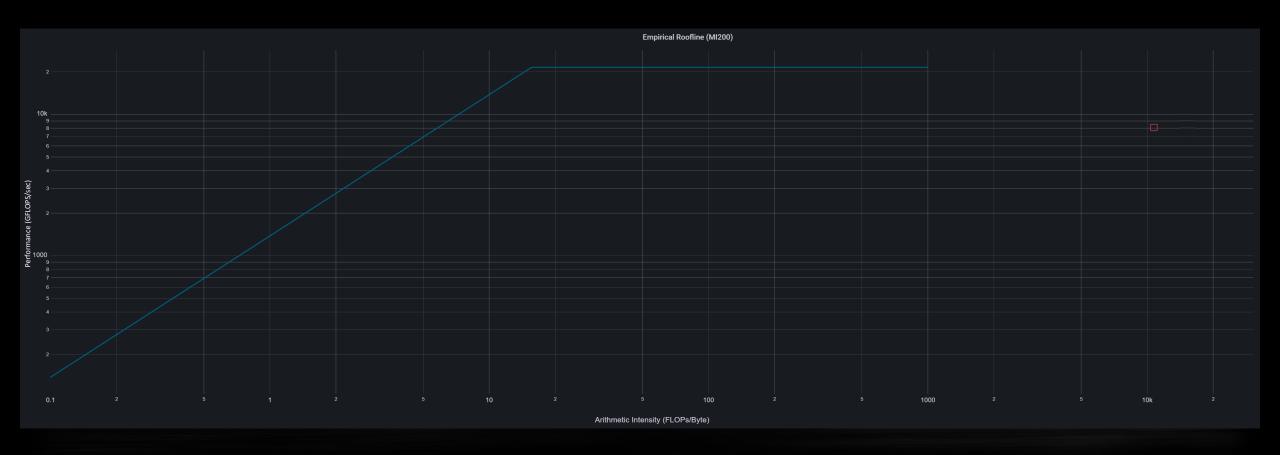
- "orig"
 - Numerical Computing 101 unoptimized implementation
- O(n²) Interaction Ops:
 - 3x V ADD
 - 6x V FMA
 - 2x V MUL
 - 1x V DIV V RSQ
 - 1x V SQRT
 - 3x RD
- O(n) Accumulation Ops:

 - 3x RD
 - 3x WR
- Interaction Al:
 - $= [(3 + 12 + 2 + 1)FLOPs / 24Bytes] * n^2 = (3/4)n^2$
- Accumulation AI:
 - (6 FLOPs / 24 Bytes) * n = n/4

```
12 typedef struct { double x, y, z, vx, vy, vz; } Body;
13
14 global
15 void bodyForce(Body *p, double dt, int n) {
    int i = blockDim.x * blockIdx.x + threadIdx.x;
     if (i < n) {
       double Fx = 0.0f; double Fy = 0.0f; double Fz = 0.0f;
18
19
20
       for (int j = 0; j < n; j++) {
21
         double dx = [p[j].x]-[p[i].x;
         double dy = p[j].y-p[i].y;
22
         double dz = p[j].z - p[i].z
23
24
         double distSqr = dx*dx + dy*dy + dz*dz + SOFTENING;
         double invDist = rsqrtf(distSqr);
25
         double invDist3 = invDist * invDist * invDist;
26
27
28
         Fx += dx * invDist3; Fy += dy * invDist3; Fz += dz * invDist3;
29
30
       [p[i].vx]+= dt*Fx; (p[i].vy] += dt*Fy; (p[i].vz) += dt*Fz;
31
33 }
```

- "orig"
 - Numerical Computing 101 unoptimized implementation

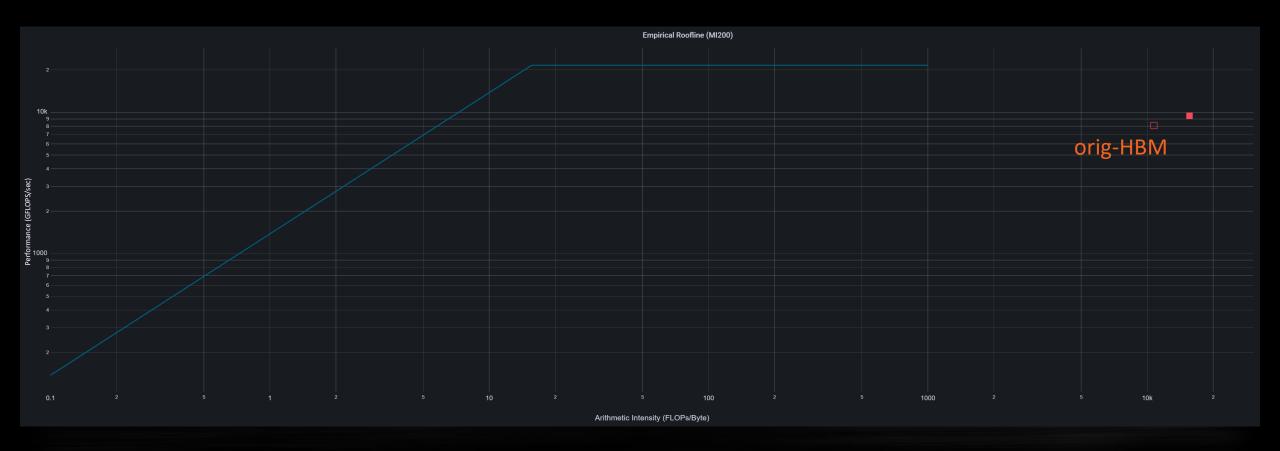
- Nbody has a very high arithmetic intensity and therefore closer to the top of the roofline (compute sensitive)
- Transcendentals like RSQ do not complete at same rate as ADD, MUL and FMA and therefore limit the peak FLOPS/s performance



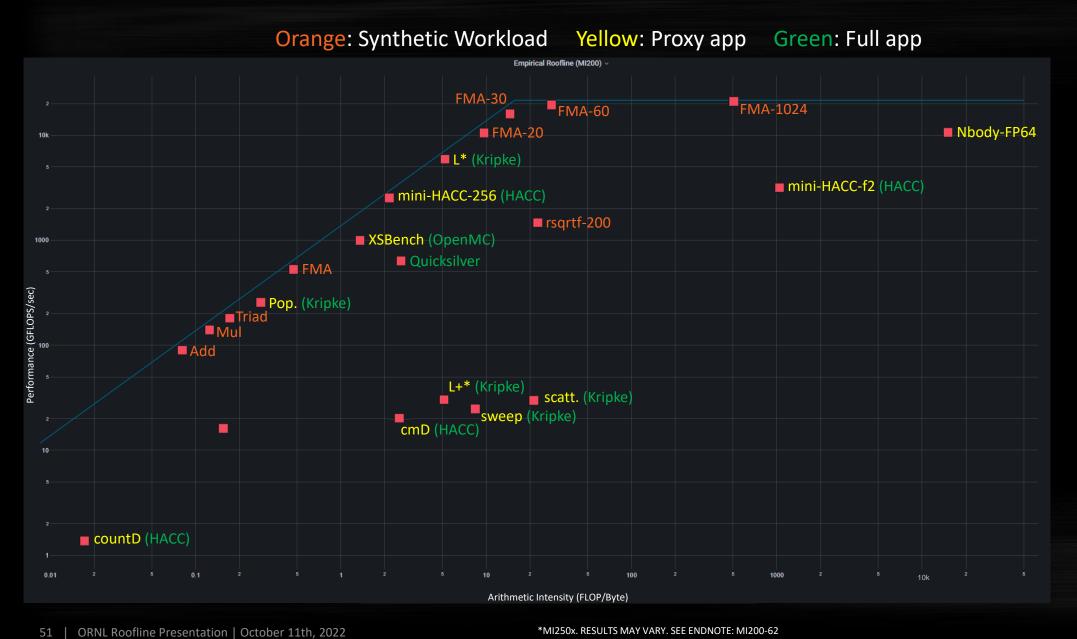
- "block"
 - Preload a "tile" size worth of particle data into faster shared memory for computing O(n2) forces
- Processing in "tiles" improves reuse and increases cache hits

```
12 typedef struct { double4 *pos, *vel; } BodySystem;
13
14 global
15 void bodyForce(double4 *p, double4 *v, double dt, int n) {
     int i = blockDim.x * blockIdx.x + threadIdx.x;
17
    if (i < n) {
18
       double Fx = 0.0f; double Fy = 0.0f; double Fz = 0.0f;
19
      for (int tile = 0; tile < gridDim.x; tile++) {</pre>
20
21
         shared double3 spos[BLOCK SIZE];
         double4 tpos = p[tile * blockDim.x + threadIdx.x];
22
23
         spos[threadIdx.x] = make double3(tpos.x, tpos.y, tpos.z);
         syncthreads();
24
25
26
         for (int j = 0; j < BLOCK_SIZE; j++) {</pre>
27
           double dx = spos[j].x - p[i].x;
           double dy = spos[j].y - p[i].y;
28
           double dz = spos[j].z - p[i].z;
29
           double distSqr = dx*dx + dy*dy + dz*dz + SOFTENING;
30
31
           double invDist = rsqrtf(distSqr);
           double invDist3 = invDist * invDist * invDist;
32
33
34
           Fx += dx * invDist3; Fy += dy * invDist3; Fz += dz * invDist3;
35
36
         syncthreads();
37
38
       v[i].x += dt*Fx; v[i].y += dt*Fy; v[i].z += dt*Fz;
39
40
41 }
```

- "block"
 - Loading and computing particle data in "tiles" to increase cache hits
- Working on smaller "tiles" of particles improves cache hits, removing loads from HBM and increasing FLOPs performance



Roofline – All Workloads



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Math Kernel Endnotes

MI200-57 - Testing Conducted by AMD performance lab as of 4/19/2022 on a single socket optimized 3rd Gen AMD EPYC™ CPU powered server with 1x AMD Instinct™ MI250X OAM (128 GB HBM2e) 560W GPU with AMD Infinity Fabric™ technology resulted in a median score of 92.6 GFLOPS/s on Add Kernel. Server manufacturers may vary configurations, yielding different results. Performance may vary based on use of latest drivers and optimizations MI200-57

MI200-58 - Testing Conducted by AMD performance lab as of 4/19/2022 on a single socket optimized 3rd Gen AMD EPYC™ CPU powered server with 1x AMD Instinct™ MI250X OAM (128 GB HBM2e) 560W GPU with AMD Infinity Fabric™ technology resulted in a median score of 149.8 GFLOPS/s on Mul Kernel. Server manufacturers may vary configurations, yielding different results. Performance may vary based on use of latest drivers and optimizations MI200-58

MI200-59 - Testing Conducted by AMD performance lab as of 4/19/2022 on a single socket optimized 3rd Gen AMD EPYC™ CPU powered server with 1x AMD Instinct™ MI250X OAM (128 GB HBM2e) 560W GPU with AMD Infinity Fabric™ technology resulted in a median score of 184.7 GFLOPS/s on Triad Kernel. Server manufacturers may vary configurations, yielding different results. Performance may vary based on use of latest drivers and optimizations MI200-59

MI200-60 - Testing Conducted by AMD performance lab as of 4/19/2022 on a single socket optimized 3rd Gen AMD EPYC™ CPU powered server with 1x AMD Instinct™ MI250X OAM (128 GB HBM2e) 560W GPU with AMD Infinity Fabric™ technology resulted in a median score of up to 21.7 TFLOPS/s on FMA Kernel. Server manufacturers may vary configurations, yielding different results. Performance may vary based on use of latest drivers and optimizations MI200-60



Nbody Endnotes

MI200-61 - Testing Conducted by AMD performance lab as of 4/19/2022 on a single socket optimized 3rd Gen AMD EPYC™ CPU powered server with 1x AMD Instinct™ MI250X OAM (128 GB HBM2e) 560W GPU with AMD Infinity Fabric™ technology resulted in a median score of 8.7 TFLOPS/s on benchmark mini-nbody-orig. Information on mini-nbody-orig: https://github.com/ROCm-Developer-Tools/HIP-Examples/blob/master/mini-nbody/hip/nbody-orig.cpp. Server manufacturers may vary configurations, yielding different results. Performance may vary based on use of latest drivers and optimizations MI200-61

MI200-62 - Testing Conducted by AMD performance lab as of 4/19/2022 on a single socket optimized 3rd Gen AMD EPYC™ CPU powered server with 1x AMD Instinct™ MI250X OAM (128 GB HBM2e) 560W GPU with AMD Infinity Fabric™ technology resulted in a median score of 9.5 TFLOPS/s on benchmark mini-nbody-block. Information on mini-nbody-block: https://github.com/ROCm-Developer-Tools/HIP-Examples/blob/master/mini-nbody/hip/nbody-block.cpp. . Server manufacturers may vary configurations, yielding different results. Performance may vary based on use of latest drivers and optimizations MI200-62





#