

Performance Tuning of Scientific Codes with the Roofline Model

1:30pm	Introductions / Administration	all
1:35pm	Roofline Introduction	Samuel Williams
2:10pm	CARM / Energy / GPUs	Aleksandar Ilic
2:40pm	Intel Advisor Installation	Zakhar Matveev
3:00pm	coffee break	
3:30pm	Introduction to Intel Advisor	Zakhar Matveev
3:45pm	Hands-on with Intel Advisor	all
4:30pm	HPC Application Studies	Charlene Yang
4:55pm	closing remarks / Q&A	all



Introductions

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Materials:

USB / Downloads

more Roofline at SC'18...

**P3HPC
Workshop**

**Friday
8:30am
D174**

“An Empirical Roofline Methodology for Quantitatively Assessing Performance Portability”, Yang, Gayatri, Kurth, Basu, Ronaghi, Adetokunbo, Friesen, Cook, Doerfler, Olikar, Deslippe, Williams

Don't forget to take the Survey...

<http://bit.ly/sc18-eval>



Introduction to the Roofline Model

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Acknowledgements

- This material is based upon work supported by the Advanced Scientific Computing Research Program in the U.S. Department of Energy, Office of Science, under Award Number DE-AC02-05CH11231.
- This material is based upon work supported by the DOE RAPIDS SciDAC Institute.
- This research used resources of the National Energy Research Scientific Computing Center (NERSC), which is supported by the Office of Science of the U.S. Department of Energy under contract DE-AC02-05CH11231.



Background

Why Use Performance Models or Tools?

- Identify performance bottlenecks
- Motivate software optimizations
- **Determine when we're done optimizing**
 - Assess performance relative to machine capabilities
 - Motivate need for algorithmic changes
- Predict performance on future machines / architectures
 - Sets realistic expectations on performance for future procurements
 - Used for HW/SW Co-Design to ensure future architectures are well-suited for the computational needs of today's applications.

Performance Models

- Many different components can contribute to kernel run time.
- Some are application-specific, and some architecture-specific.

#FP operations	Flop/s
Cache data movement	Cache GB/s
DRAM data movement	DRAM GB/s
PCIe data movement	PCIe bandwidth
Depth	OMP Overhead
MPI Message Size	Network Bandwidth
MPI Send:Wait ratio	Network Gap
#MPI Wait's	Network Latency

Performance Models

- Can't think about all these terms all the time for every application...

Computational
Complexity

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Performance Models

- Because there are so many components, performance models often conceptualize the system as being dominated by one or more of these components.

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LogP

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LogGP

Alexandrov, et al, "LogGP: incorporating long messages into the LogP model - one step closer towards a realistic model for parallel computation", SPAA, 1995.

Performance Models

- Because there are so many components, performance models often conceptualize the system as being dominated by one or more of these components.

#FP operations	Flop/s	Roofline Model
Cache data movement	Cache GB/s	
DRAM data movement	DRAM GB/s	
PCIe data movement	PCIe bandwidth	
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Roofline Model:

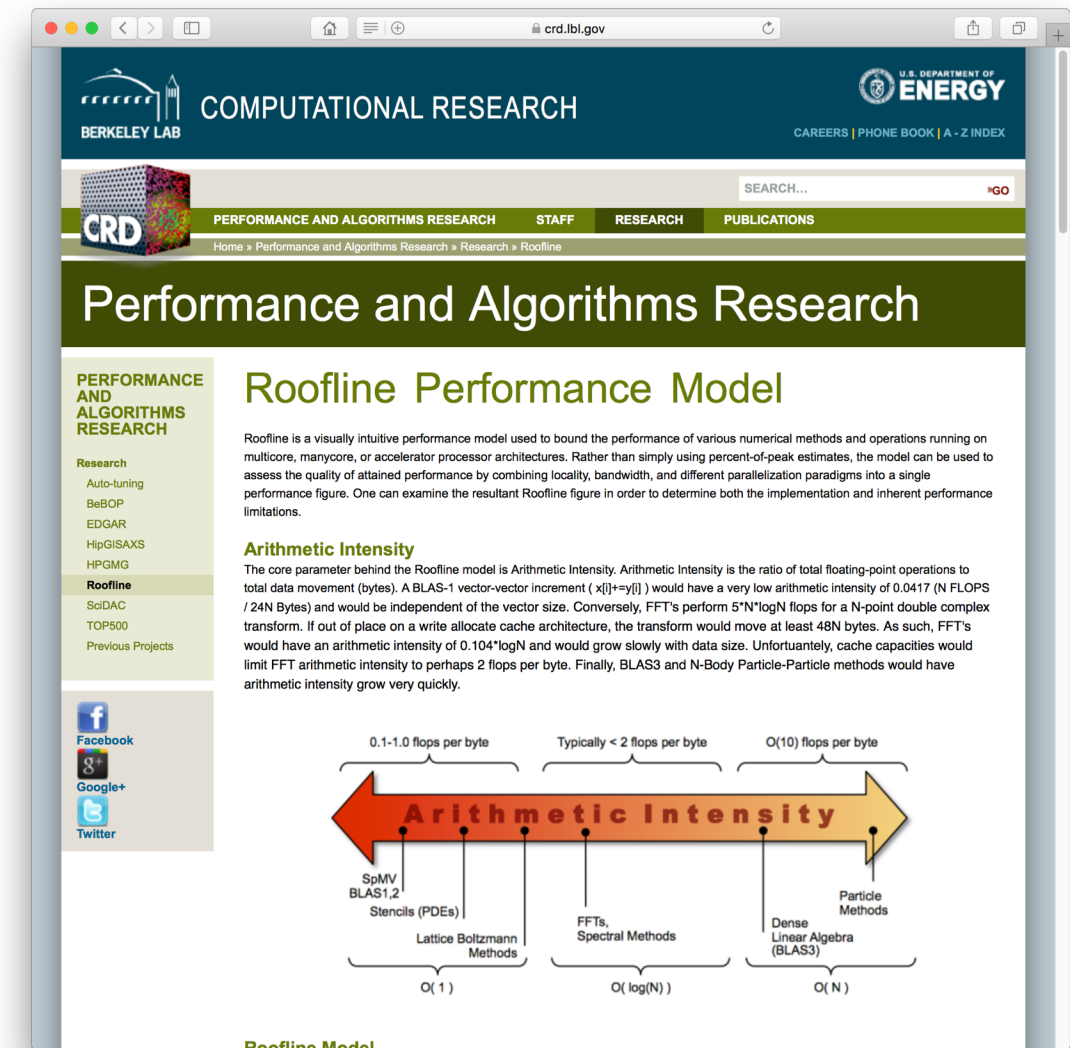
Arithmetic Intensity and Bandwidth

Performance Models / Simulators

- Historically, many performance models and simulators tracked time to predict performance (i.e. counting cycles)
- The last two decades saw a number of latency-hiding techniques...
 - Out-of-order execution (hardware discovers parallelism to hide latency)
 - HW stream prefetching (hardware speculatively loads data)
 - Massive thread parallelism (independent threads satisfy the latency-bandwidth product)
- ... resulted in a shift from a latency-limited computing regime to a **throughput-limited computing regime**

Roofline Model

- **Roofline Model** is a throughput-oriented performance model...
 - Tracks rates not times
 - Augmented with Little's Law
(concurrency = latency*bandwidth)
 - Independent of ISA and architecture (applies to CPUs, GPUs, Google TPUs¹, etc...)

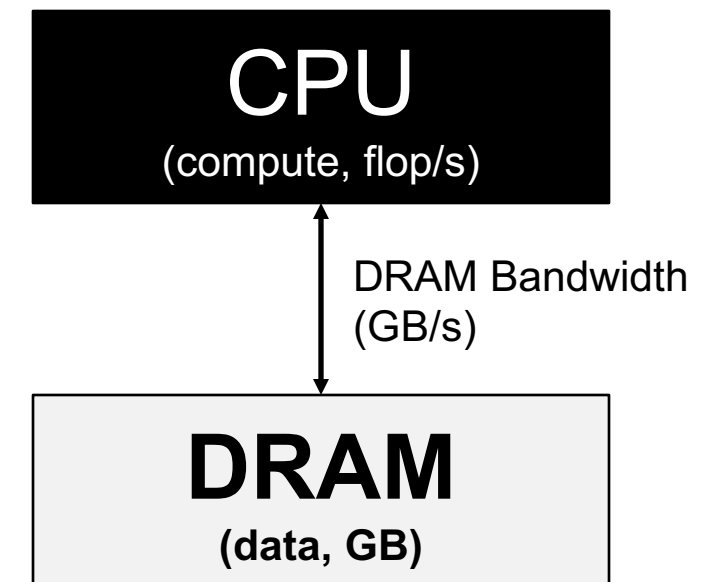


<https://crd.lbl.gov/departments/computer-science/PAR/research/roofline>

¹Jouppi et al, "In-Datacenter Performance Analysis of a Tensor Processing Unit", ISCA, 2017.

(DRAM) Roofline

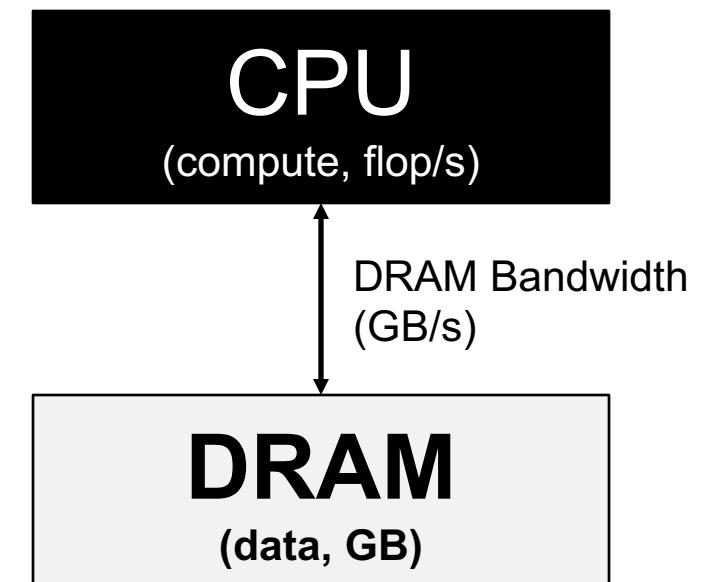
- One could hope to always attain peak performance (Flop/s)
- However, finite reuse and bandwidth limit performance.
- Assuming perfect overlap of communication and computation...



$$\text{Time} = \max \left\{ \begin{array}{l} \text{\#FP ops} / \text{Peak GFlop/s} \\ \text{\#Bytes} / \text{Peak GB/s} \end{array} \right.$$

(DRAM) Roofline

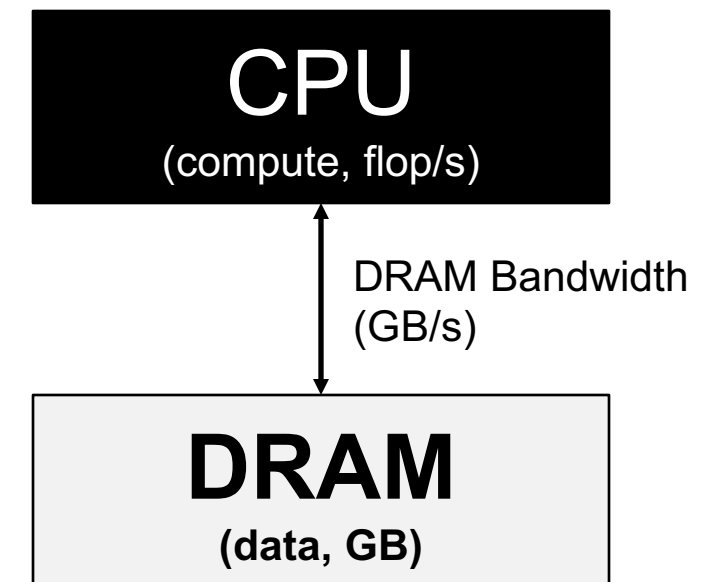
- One could hope to always attain peak performance (Flop/s)
- However, finite reuse and bandwidth limit performance.
- Assuming perfect overlap of communication and computation...



$$\frac{\text{Time}}{\text{\#FP ops}} = \max \begin{cases} 1 / \text{Peak GFlop/s} \\ \text{\#Bytes} / \text{\#FP ops} / \text{Peak GB/s} \end{cases}$$

(DRAM) Roofline

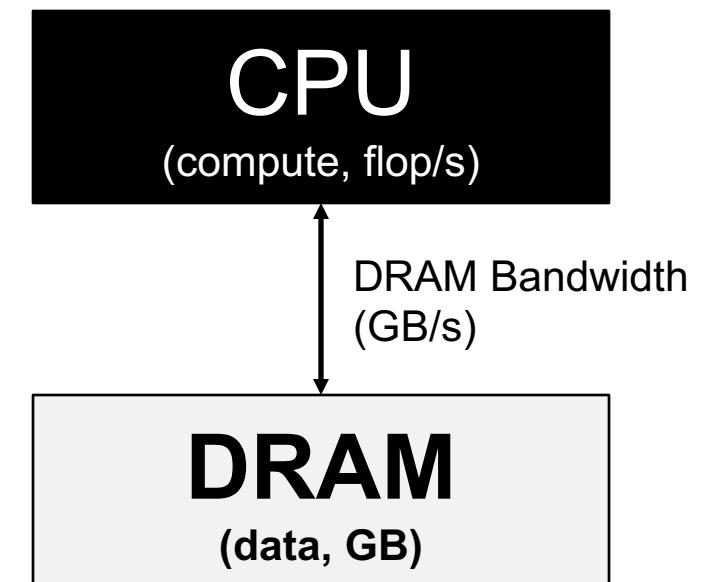
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- Assuming perfect overlap of communication and computation...



$$\frac{\text{\#FP ops}}{\text{Time}} = \min \left\{ \begin{array}{l} \text{Peak GFlop/s} \\ (\text{\#FP ops} / \text{\#Bytes}) * \text{Peak GB/s} \end{array} \right.$$

(DRAM) Roofline

- One could hope to always attain peak performance (Flop/s)
- However, finite reuse and bandwidth limit performance.
- Assuming perfect overlap of communication and computation...

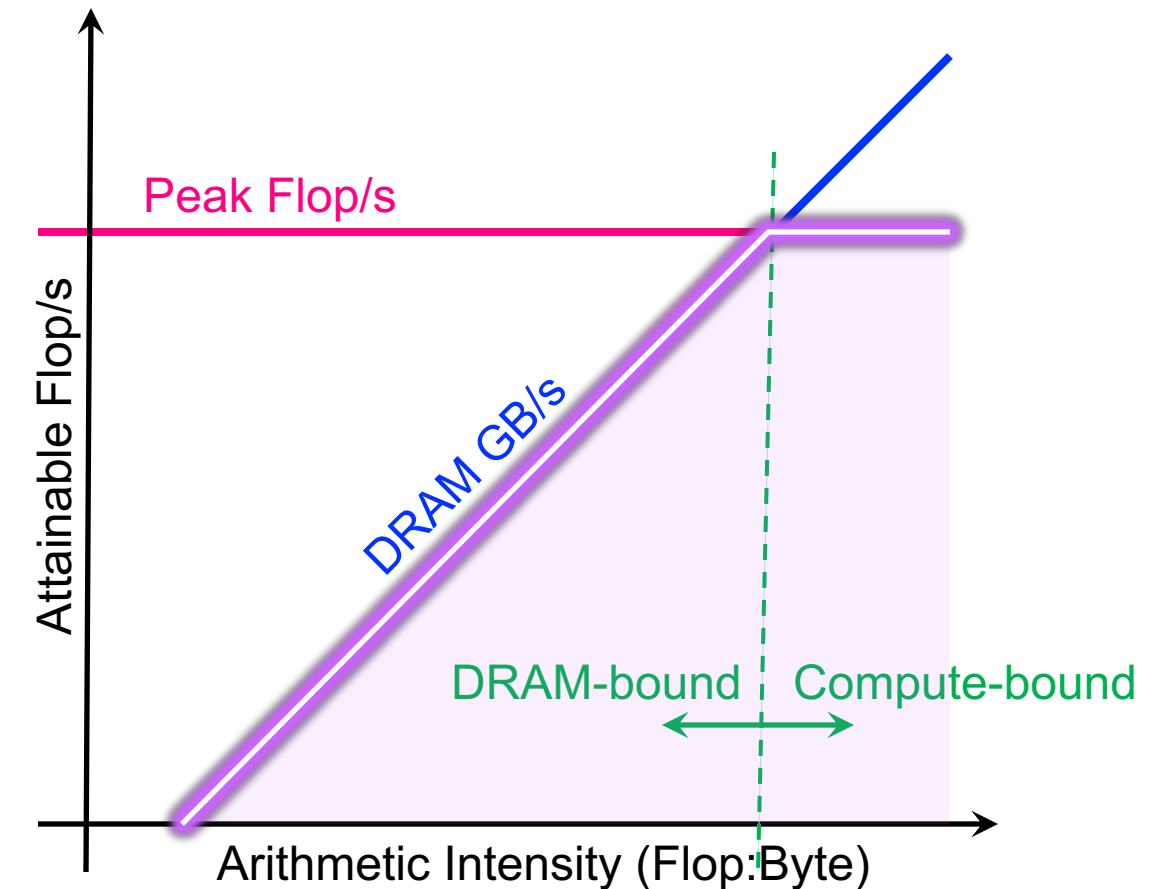


$$\text{GFlop/s} = \min \begin{cases} \text{Peak GFlop/s} \\ \text{AI} * \text{Peak GB/s} \end{cases}$$

Note, Arithmetic Intensity (AI) = Flops / Bytes (as presented to DRAM)

(DRAM) Roofline

- Plot Roofline bound using Arithmetic Intensity as the x-axis
- **Log-log scale** makes it easy to doodle, extrapolate performance along Moore's Law, etc...
- Kernels with AI less than machine balance are ultimately DRAM bound (we'll refine this later...)

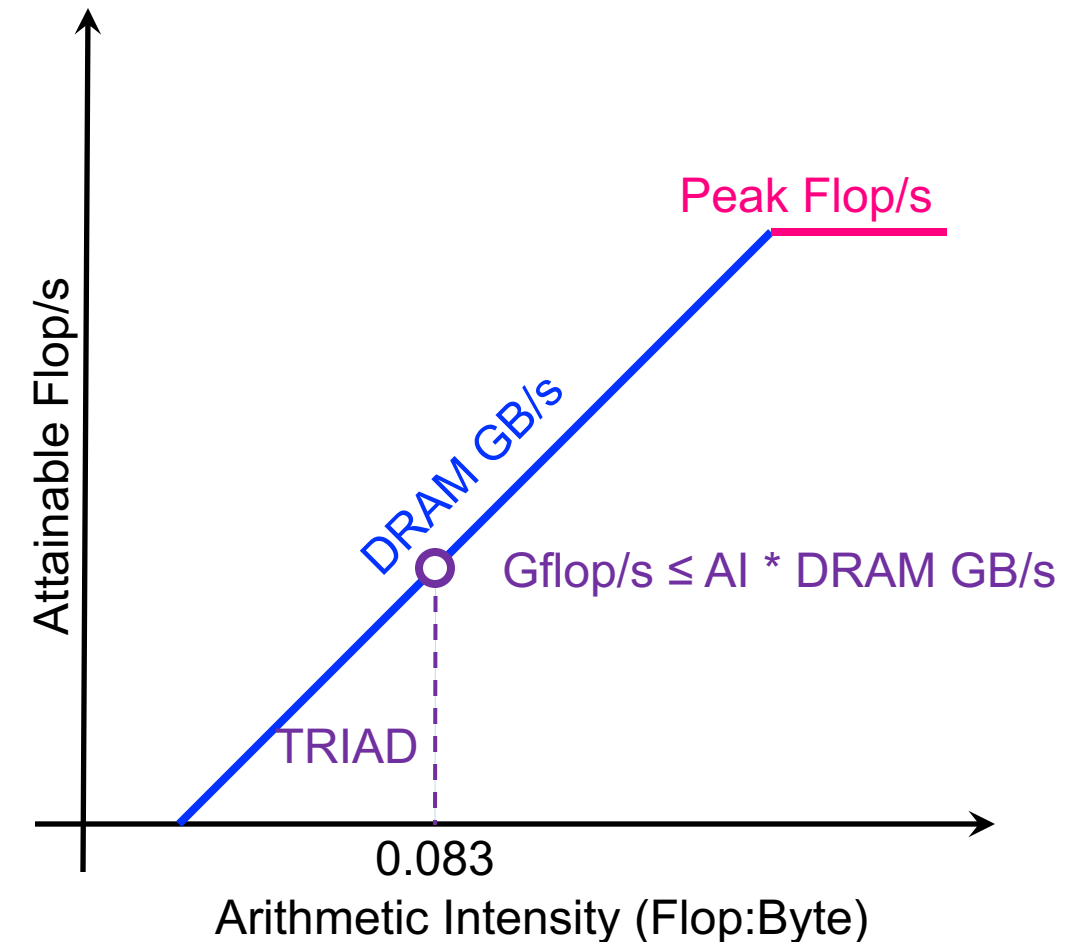


Roofline Example #1

- Typical machine balance is 5-10 flops per byte...
 - 40-80 flops per double to exploit compute capability
 - Artifact of technology and money
 - **Unlikely to improve**
- Consider STREAM Triad...

```
#pragma omp parallel for
for(i=0;i<N;i++){
    z[i] = x[i] + alpha*y[i];
}
```

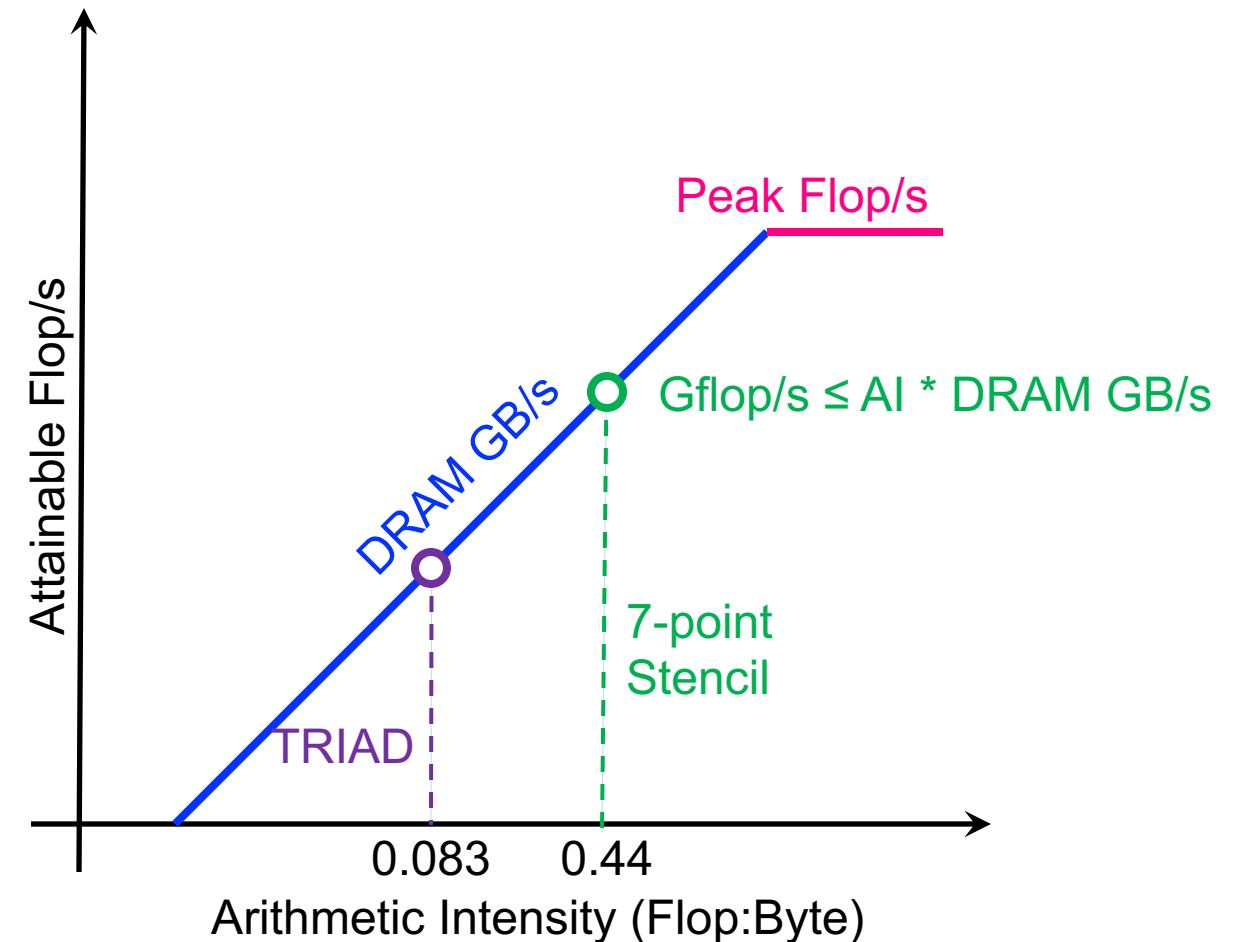
 - 2 flops per iteration
 - Transfer 24 bytes per iteration (read X[i], Y[i], write Z[i])
 - **AI = 0.083 flops per byte == Memory bound**



Roofline Example #2

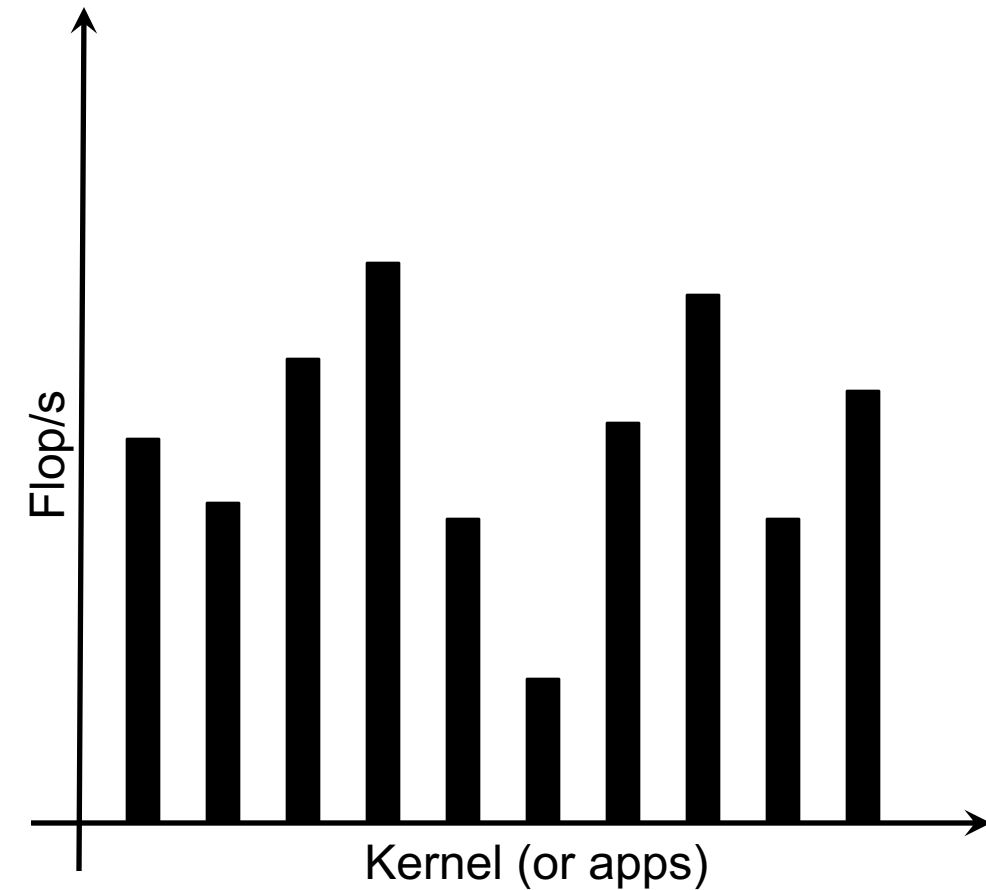
- Conversely, 7-point constant coefficient stencil...
 - 7 flops
 - 8 memory references (7 reads, 1 store) per point
 - Cache can filter all but 1 read and 1 write per point
 - **AI = 0.44 flops per byte == memory bound, but 5x the flop rate**

```
#pragma omp parallel for
for(k=1;k<dim+1;k++){
for(j=1;j<dim+1;j++){
for(i=1;i<dim+1;i++){
    new[k][j][i] = -6.0*old[k][j][i]
                  + old[k][j][i-1]
                  + old[k][j][i+1]
                  + old[k][j-1][i]
                  + old[k][j+1][i]
                  + old[k-1][j][i]
                  + old[k+1][j][i];
}}}
```



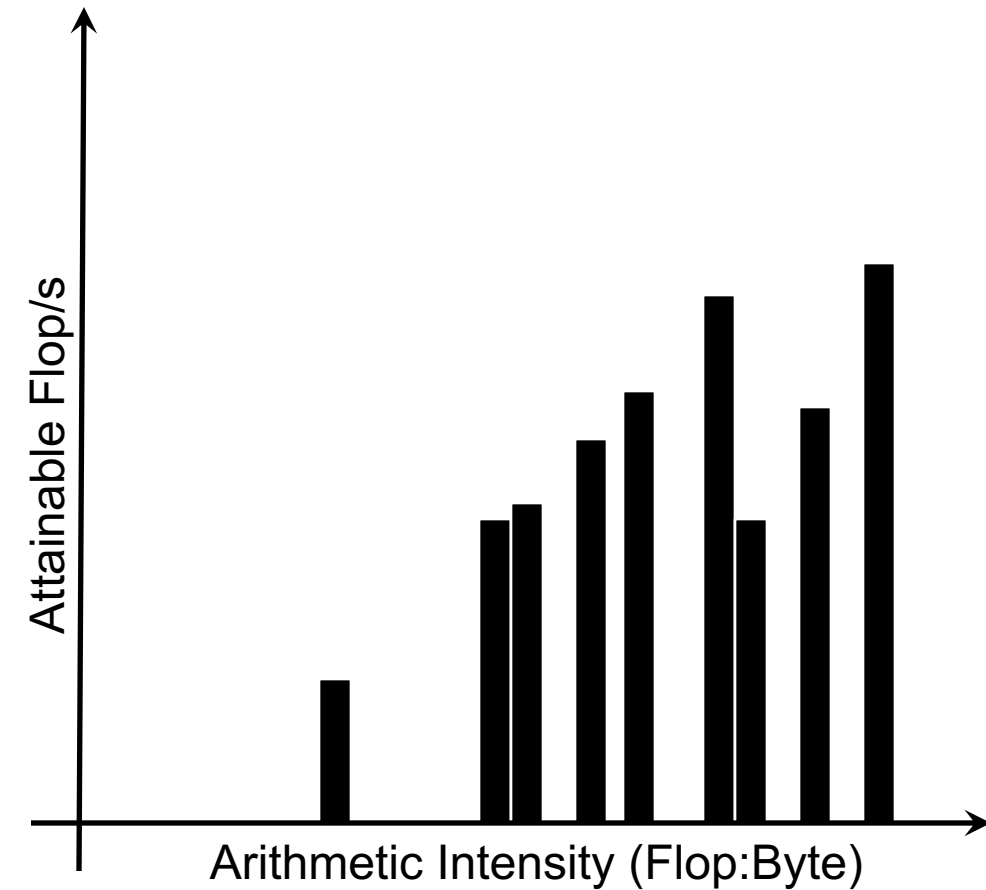
Why is Roofline Useful?

- Imagine a mix of loop nests
- Flop/s alone may not be useful in deciding which to optimize first



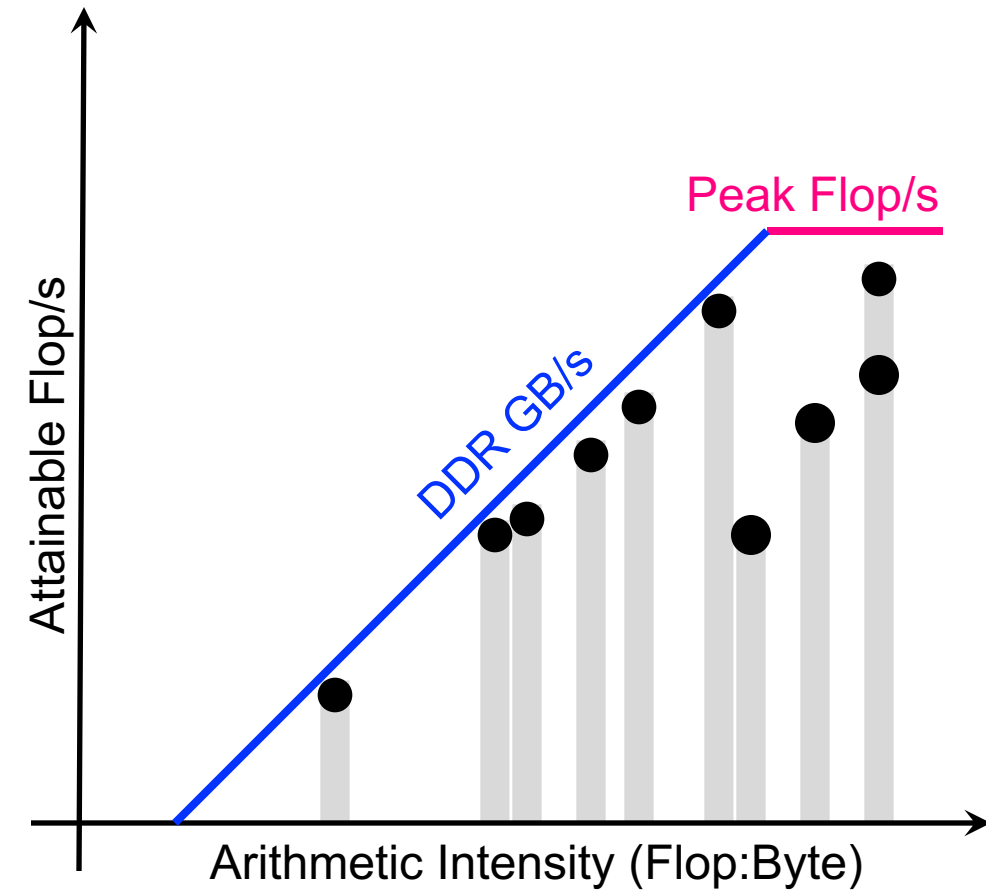
Why is Roofline Useful?

- We can sort kernels by AI ...



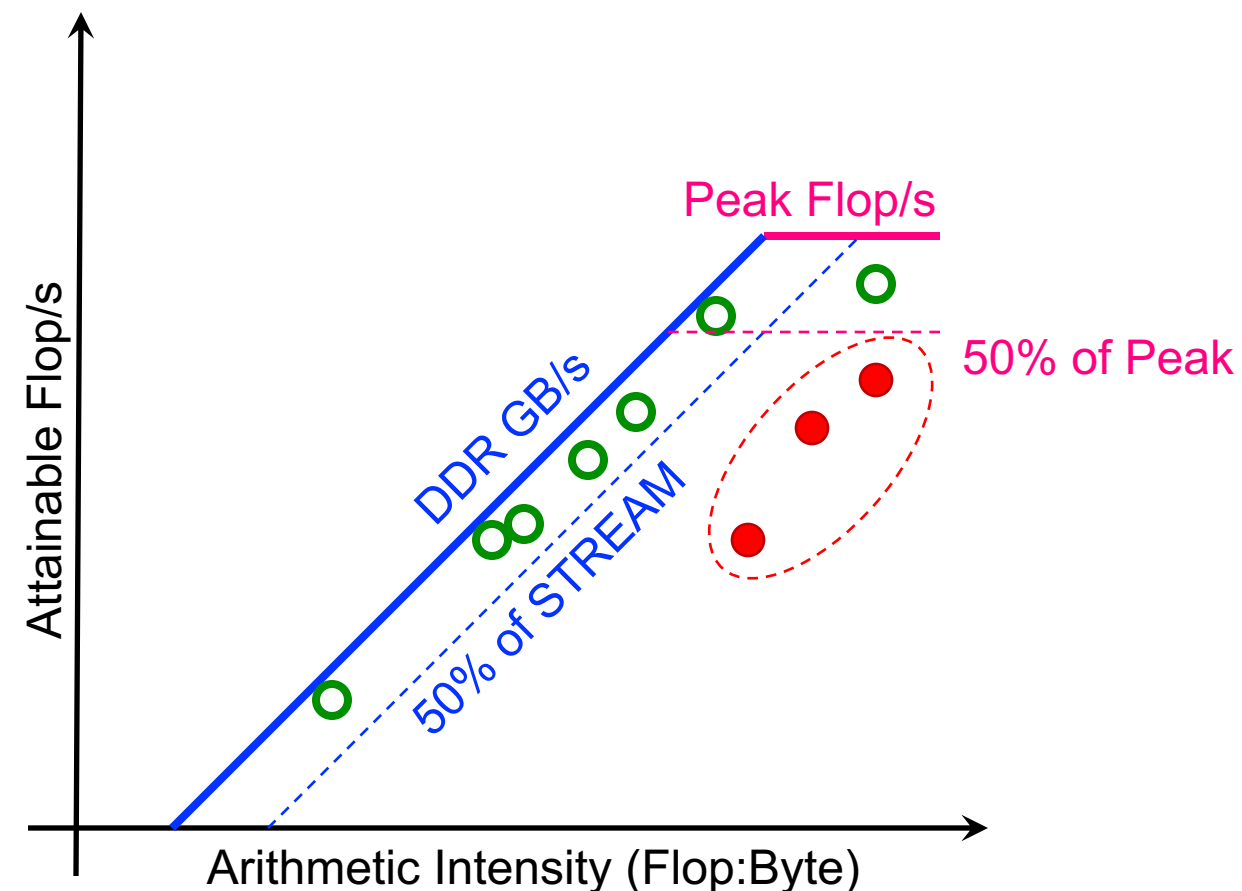
Why is Roofline Useful?

- We can sort kernels by AI ...
- ... and compare performance relative to machine capabilities



Why is Roofline Useful?

- Kernels near the roofline are making good use of computational resources
 - kernels can have low performance (Gflop/s), but make good use of a machine
 - kernels can have high performance (Gflop/s), but make poor use of a machine



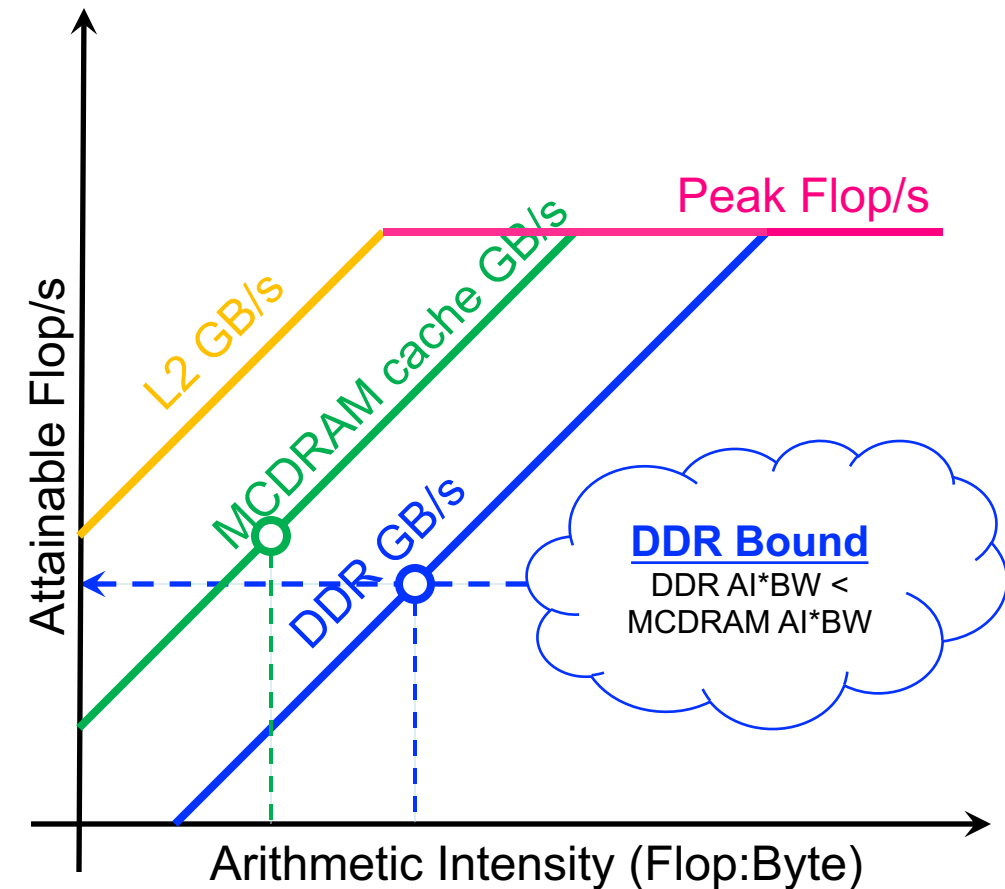
Refining Roofline: Memory Hierarchy & DLP

Hierarchical Roofline

- Processors have multiple levels of memory/cache
 - Registers
 - L1, L2, L3 cache
 - MCDRAM/HBM (KNL/GPU device memory)
 - DDR (main memory)
 - NVRAM (non-volatile memory)
- Applications have locality in each level
 - Unique data movements imply unique AI's
 - Moreover, each level will have a unique bandwidth

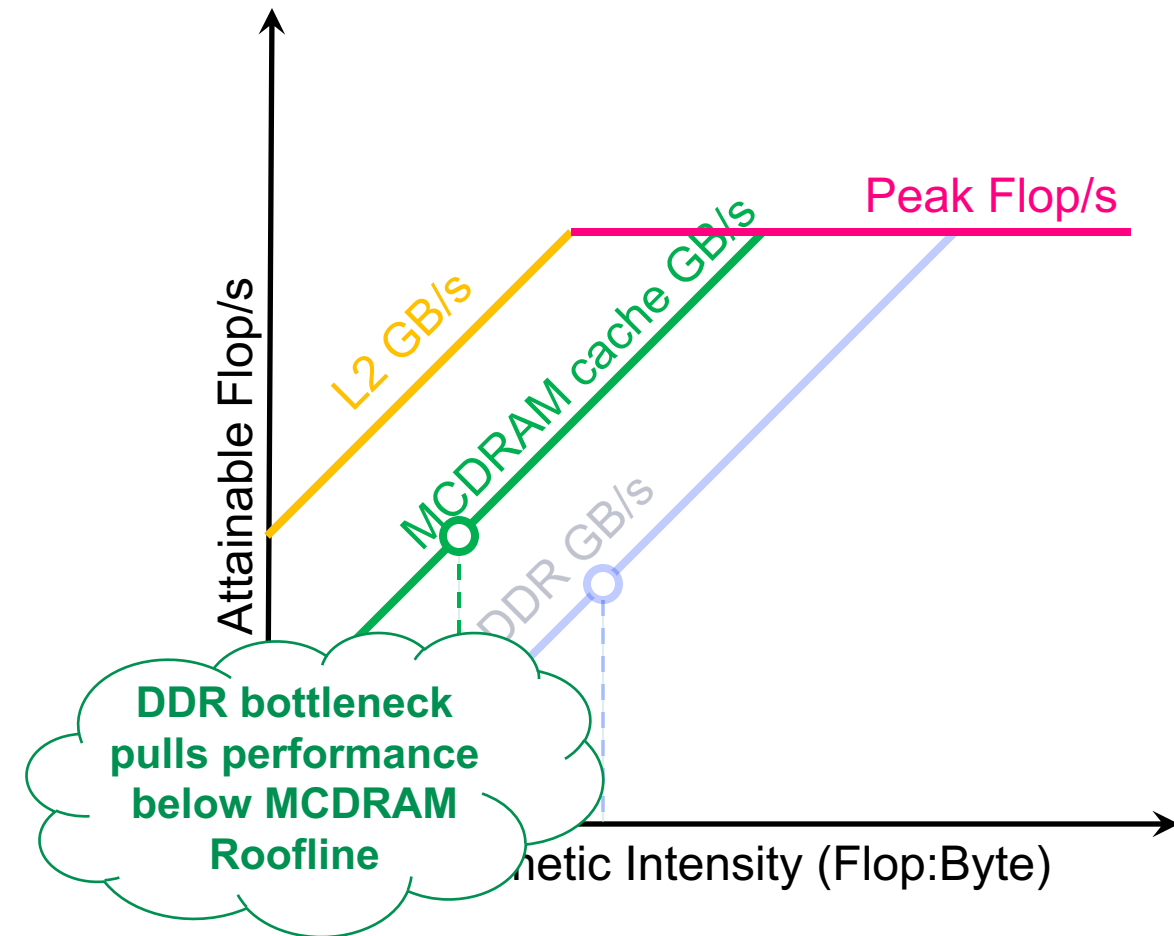
Hierarchical Roofline

- Construct superposition of Rooflines...
 - Measure bandwidth
 - Measure AI for each level of memory
 - Although an loop nest may have multiple AI's and multiple bounds (flops, L1, L2, ... DRAM)...
 - ... **performance is bound by the minimum**



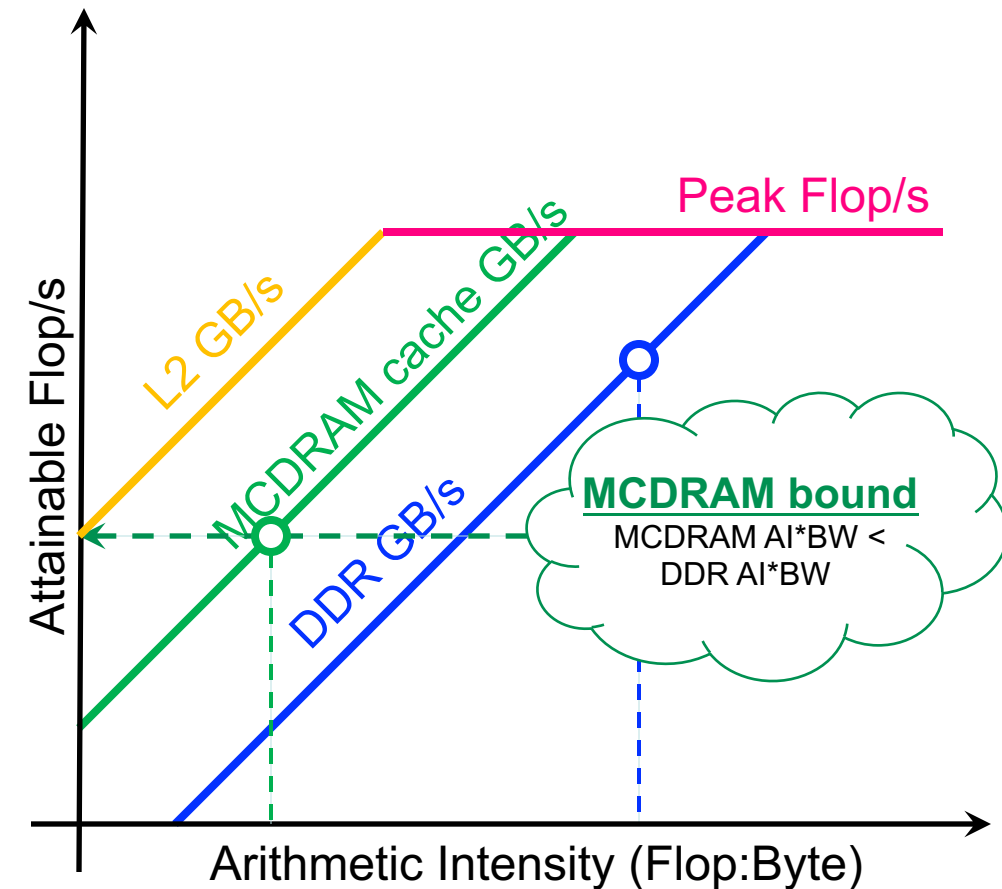
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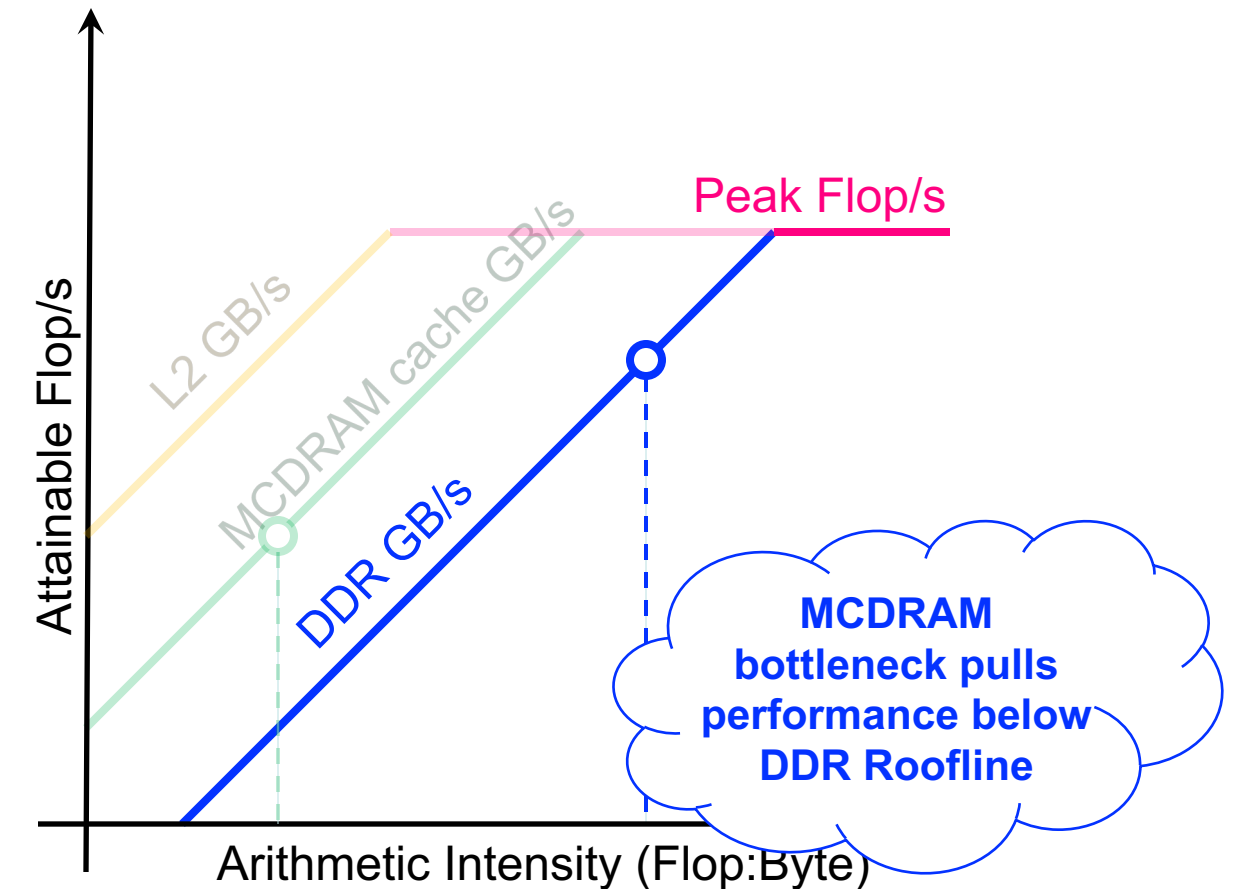
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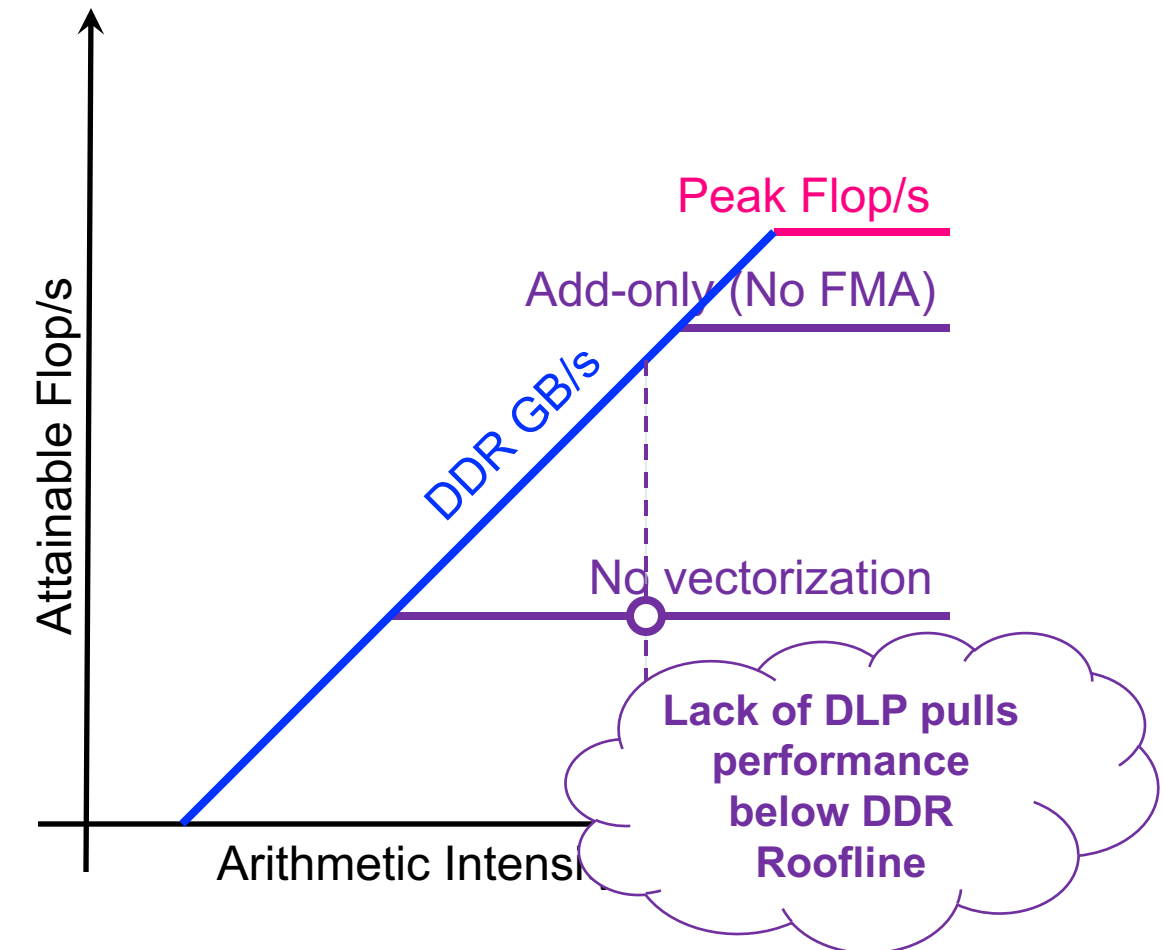
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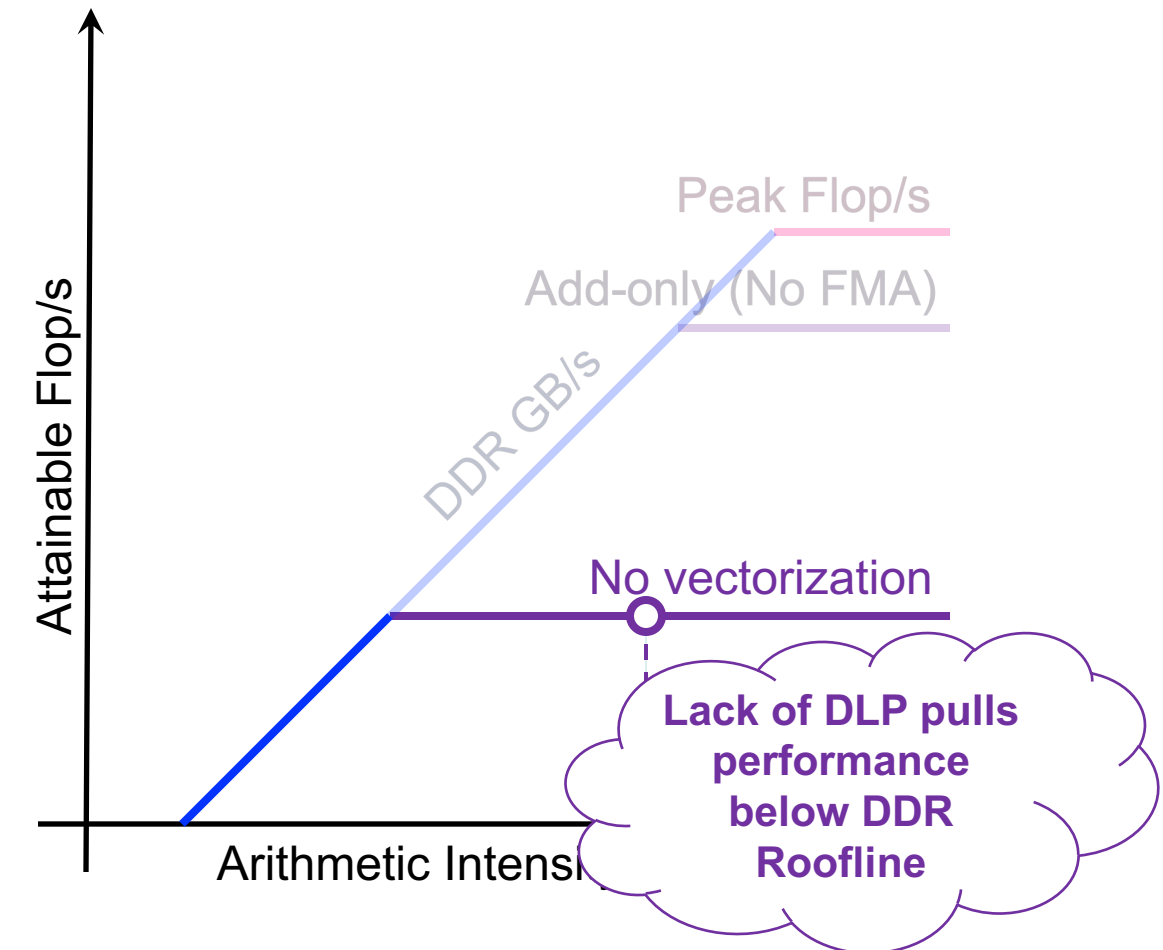
Data, Instruction, Thread-Level Parallelism...

- We have assumed one can attain peak flops with high locality.
- In reality, we must ...
 - Use special instructions (e.g. FMA)
 - Vectorize loops (16 flops per instruction)
 - Hide FPU latency (unrolling, out-of-order execution)
 - Use all cores & sockets
- Without these, ...
 - Peak performance is not attainable
 - Some kernels can transition from memory-bound to compute-bound



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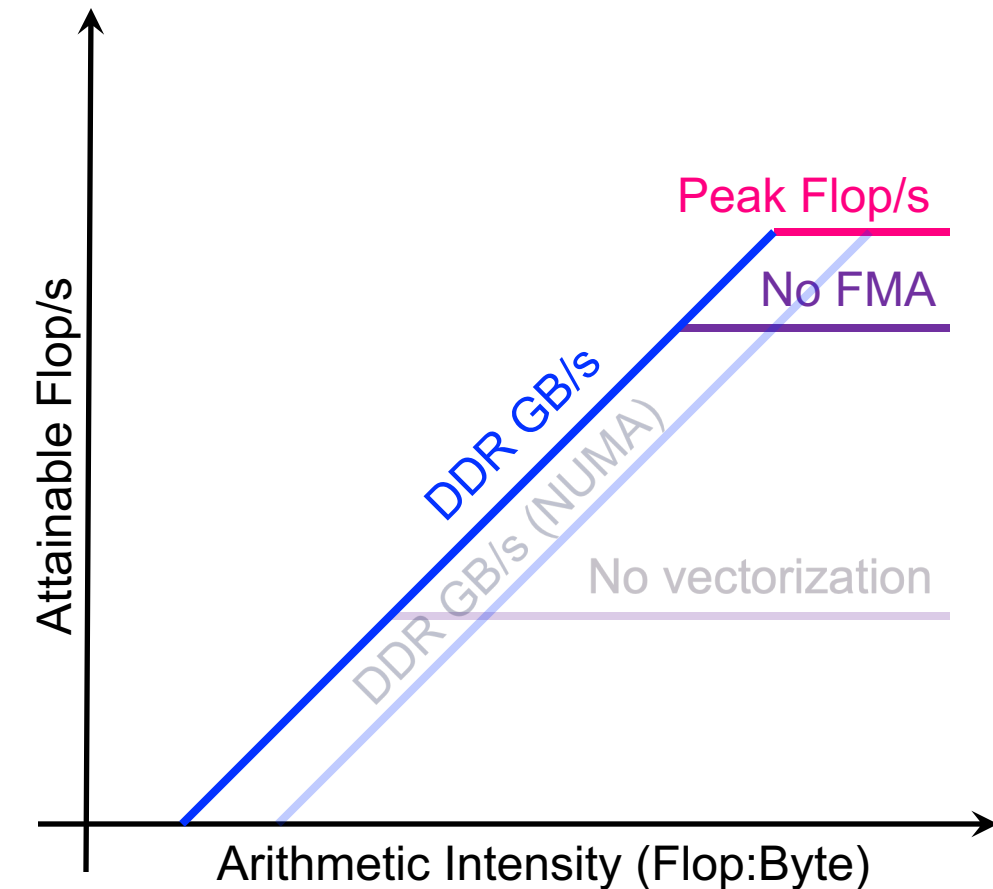


Roofline Model:

Roofline-driven Performance Optimization

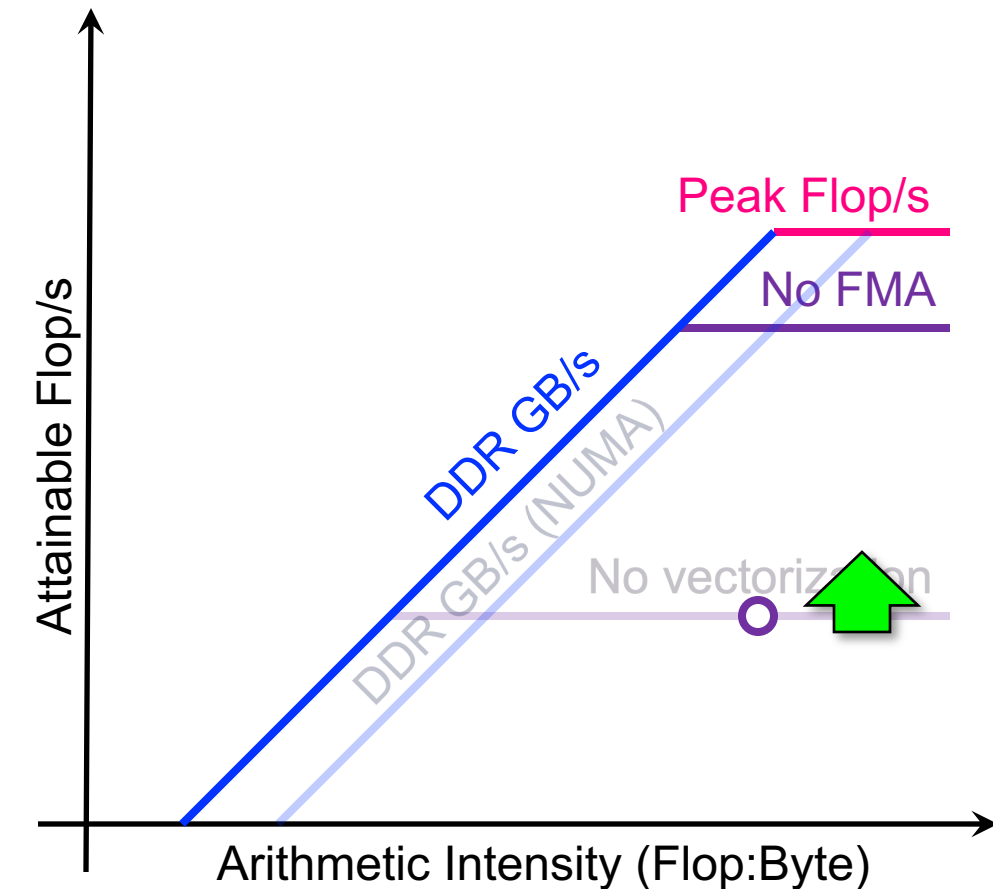
Roofline-Driven Performance Optimization

- Broadly speaking, there are three approaches to improving performance:



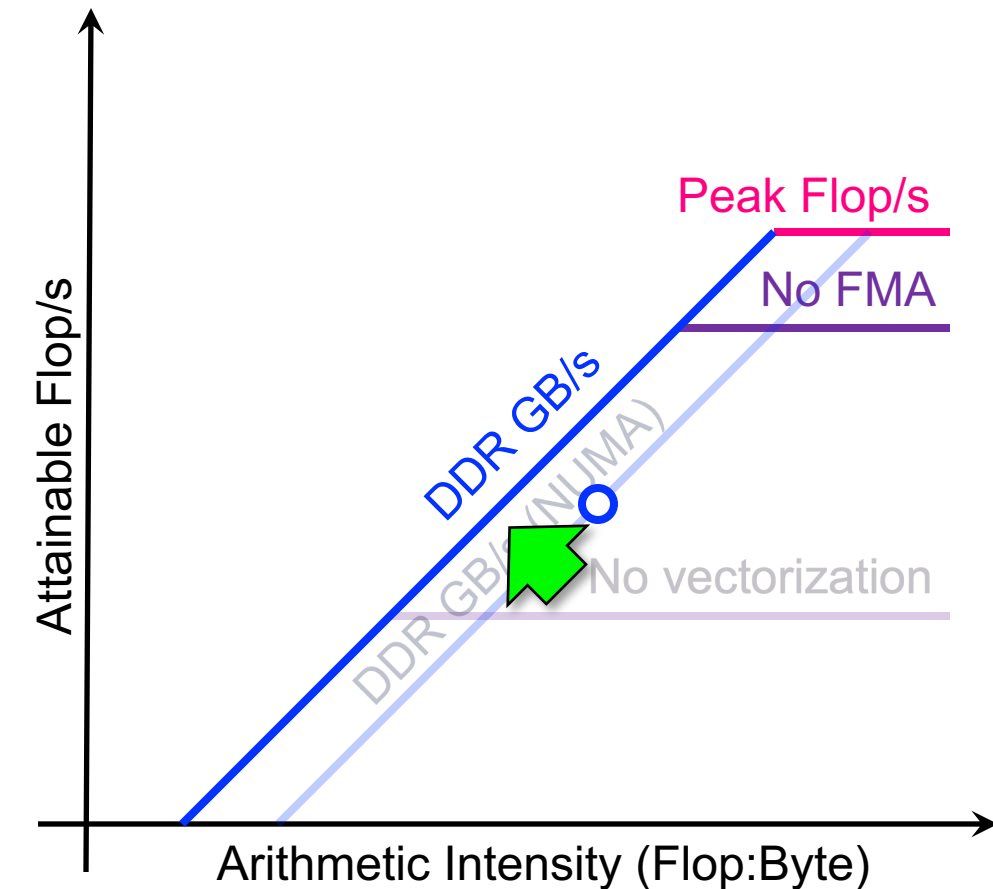
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- **Maximize in-core performance (e.g. get compiler to vectorize)**



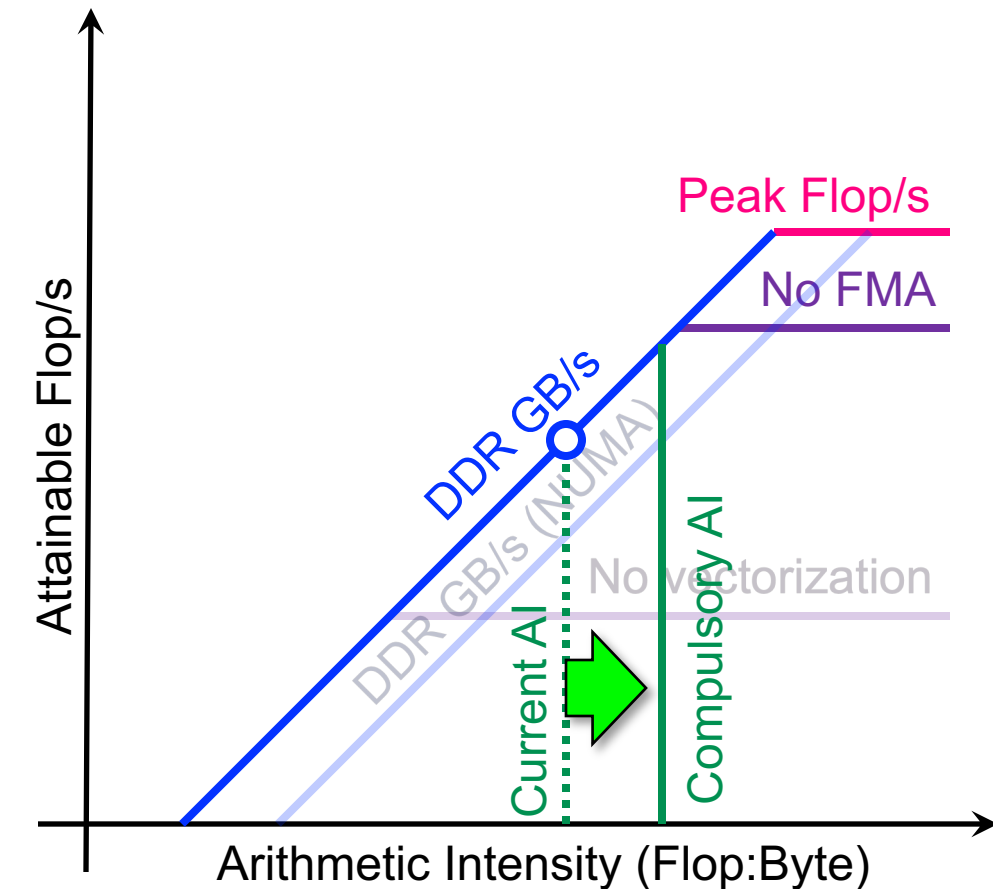
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- **Maximize memory bandwidth (e.g. NUMA-aware, unit-stride)**



Roofline-Driven Performance Optimization

- Broadly speaking, there are three approaches to improving performance:
- Maximize in-core performance (e.g. get compiler to vectorize)
- Maximize memory bandwidth (e.g. NUMA-aware, unit stride)
- **Minimize data movement (e.g. cache blocking)**



Roofline In Practice:

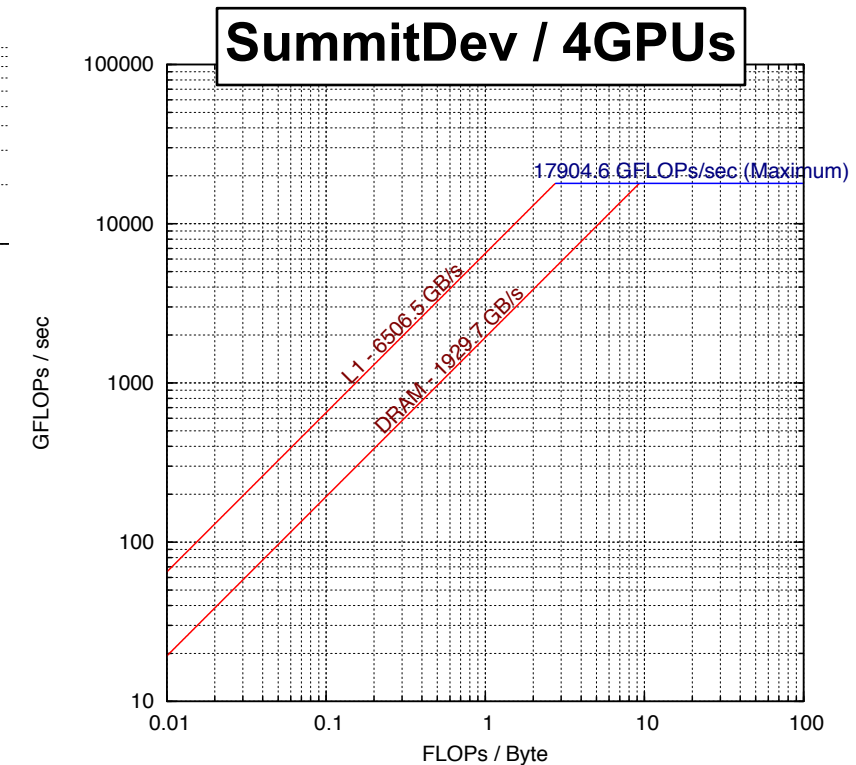
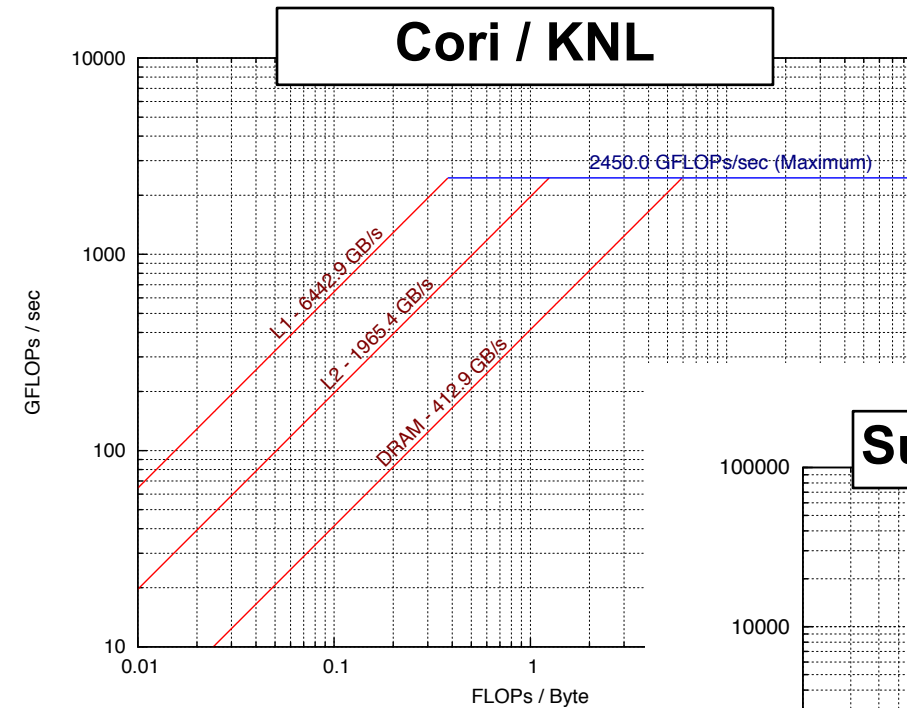
Evolution at LBL / NERSC

Step 1:

Machine Characterization

Machine Characterization

- **“Theoretical Performance”**
numbers can be highly optimistic...
 - Pin BW vs. sustained bandwidth
 - TurboMode / Underclock for AVX
 - compiler failings on high-AI loops.
- LBL developed the Empirical Roofline Toolkit (ERT)...
 - Characterize CPU/GPU systems
 - Peak Flop rates
 - Bandwidths for each level of memory
 - **MPI+OpenMP/CUDA == multiple GPUs**



Step 2:

Application Characterization

Measuring AI

- To characterize execution with Roofline we need...
 - **Time**
 - **Flops** (\Rightarrow flop's / time)
 - **Data movement** between each level of memory (\Rightarrow Flop's / GB's)
- We can look at the full application...
 - Coarse grained, 30-min average
 - Misses many details and bottlenecks
- or we can look at individual loop nests...
 - Requires auto-instrumentation on a loop by loop basis
 - Moreover, we should probably differentiate data movement or flops on a core-by-core basis.

How Do We Count Flop's?

Manual Counting

- Go thru each loop nest and count the number of FP operations
- ✓ Works best for deterministic loop bounds
- ✓ or parameterize by the number of iterations (recorded at run time)
- ✗ Not scalable

Perf. Counters

- Read counter before/after
- ✓ More Accurate
- ✓ Low overhead (<%) == can run full MPI applications
- ✓ Can detect load imbalance
- ✗ Requires privileged access
- ✗ Requires manual instrumentation (+overhead) or full-app characterization
- ✗ Broken counters = garbage
- ✗ May not differentiate FMADD from FADD
- ✗ No insight into special pipelines

Binary Instrumentation

- Automated inspection of assembly at run time
- ✓ Most Accurate
- ✓ FMA-, VL-, and mask-aware
- ✓ Can count instructions by class/type
- ✓ Can detect load imbalance
- ✓ Can include effects from non-FP instructions
- ✓ Automated application to multiple loop nests
- ✗ >10x overhead (short runs / reduced concurrency)

How Do We Measure Data Movement?

Manual Counting

- Go thru each loop nest and estimate how many bytes will be moved
- Use a mental model of caches
- ✓ Works best for simple loops that stream from DRAM (stencils, FFTs, sparse, ...)
- ✗ N/A for complex caches
- ✗ Not scalable

Perf. Counters

- Read counter before/after
- ✓ Applies to full hierarchy (L2, DRAM,
- ✓ Much more Accurate
- ✓ Low overhead (<%) == can run full MPI applications
- ✓ Can detect load imbalance
- ✗ Requires privileged access
- ✗ Requires manual instrumentation (+overhead) or full-app characterization

Cache Simulation

- Build a full cache simulator driven by memory addresses
- ✓ Applies to full hierarchy and multicore
- ✓ Can detect load imbalance
- ✓ Automated application to multiple loop nests
- ✗ Ignores prefetchers
- ✗ >10x overhead (short runs / reduced concurrency)

Previously Cobbled Together Tools...

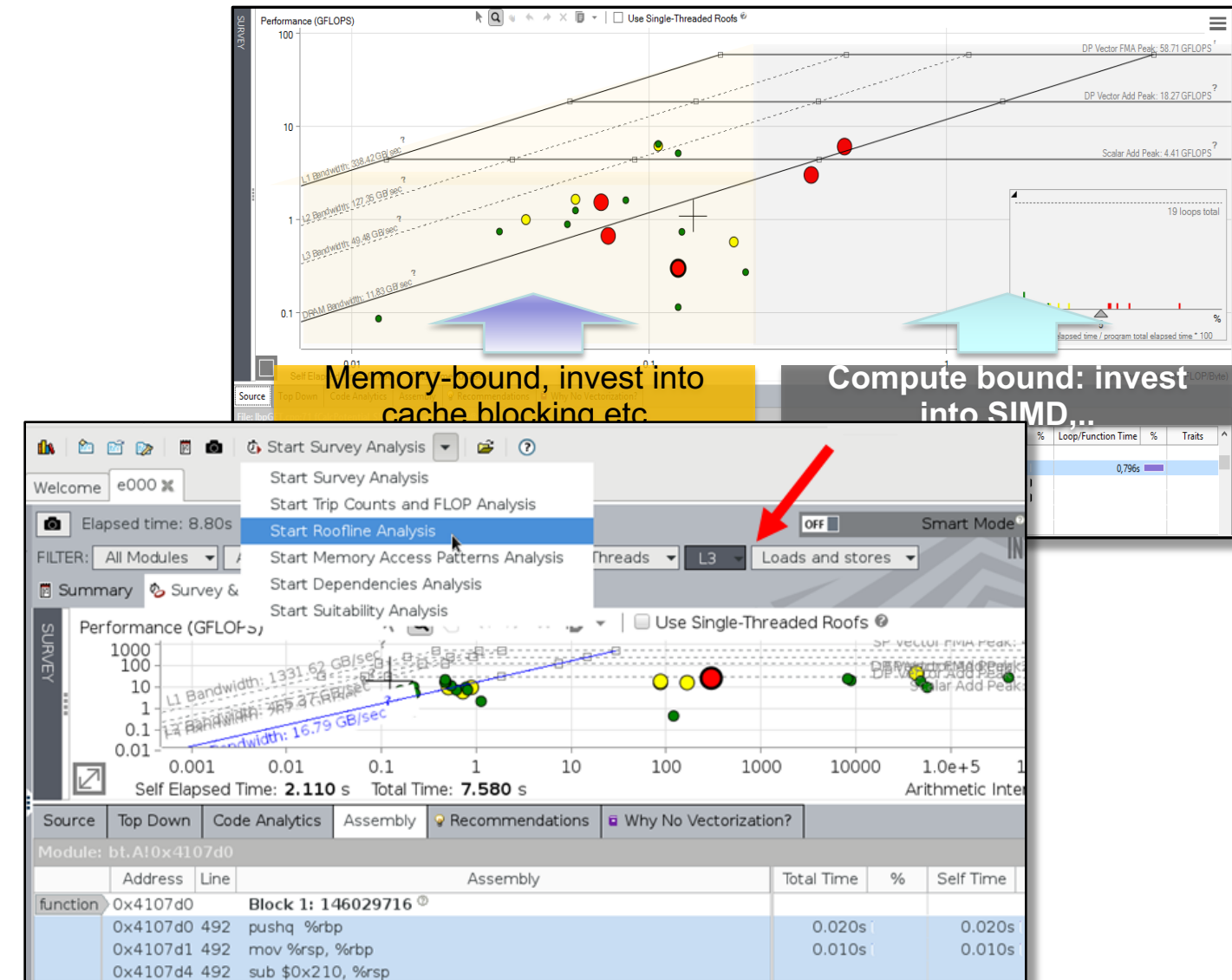
- Use tools known/observed to work on NERSC's Cori (KNL, HSW)...
 - Used **Intel SDE** (Pin binary instrumentation + emulation) to create software Flop counters
 - Used **Intel VTune** performance tool (NERSC/Cray approved) to access uncore counters
- Accurate measurement of Flop's (HSW) and DRAM data movement (HSW and KNL)
- Used by NESAP (NERSC KNL application readiness project) to characterize apps on Cori...



<http://www.nersc.gov/users/application-performance/measuring-arithmetic-intensity/>

Intel Advisor

- Includes Roofline Automation...
 - ✓ Automatically instruments applications (one dot per loop nest/function)
 - ✓ Computes FLOPS and AI for each function (**CARM**)
 - ✓ AVX-512 support that incorporates masks
 - ✓ **Integrated Cache Simulator¹** (hierarchical roofline / multiple AI's)
 - ✓ Automatically benchmarks target system (calculates ceilings)
 - ✓ Full integration with existing Advisor capabilities



<http://www.nersc.gov/users/training/events/roofline-training-1182017-1192017>

¹Experimental Feature, the look and feel and exact behavior is subject for change

Hierarchical Roofline vs. Cache-Aware Roofline

*...understanding different Roofline
formulations in Intel Advisor*

There are two Major Roofline Formulations:

- Hierarchical Roofline (original Roofline w/ DRAM, L3, L2, ...)...
 - Williams, et al, “Roofline: An Insightful Visual Performance Model for Multicore Architectures”, CACM, 2009
 - Chapter 4 of “Auto-tuning Performance on Multicore Computers”, 2008
 - Defines multiple bandwidth ceilings and multiple AI’s per kernel
 - Performance bound is the minimum of flops and the memory intercepts (superposition of original, single-metric Rooflines)
- Cache-Aware Roofline
 - Illic et al, "Cache-aware Roofline model: Upgrading the loft", IEEE Computer Architecture Letters, 2014
 - Defines multiple bandwidth ceilings, but uses a single AI (flop:L1 bytes)
 - As one loses cache locality (capacity, conflict, ...) performance falls from one BW ceiling to a lower one at constant AI
- Why Does this matter?
 - Some tools use the Hierarchical Roofline, some use cache-aware == **Users need to understand the differences**
 - Cache-Aware Roofline model was integrated into production Intel Advisor
 - Evaluation version of Hierarchical Roofline¹ (cache simulator) has also been integrated into Intel Advisor

¹Experimental Feature, the look and feel and exact behavior is subject for change

Hierarchical Roofline

- Captures cache effects
- AI is Flop:Bytes after being *filtered by lower cache levels*
- Multiple Arithmetic Intensities (one per level of memory)
- AI *dependent* on problem size (capacity misses reduce AI)
- Memory/Cache/Locality effects are *observed as decreased AI*
- Requires *performance counters or cache simulator* to correctly measure AI

Cache-Aware Roofline

- Captures cache effects
- AI is Flop:Bytes *as presented to the L1 cache (plus non-temporal stores)*
- Single Arithmetic Intensity
- AI *independent* of problem size
- Memory/Cache/Locality effects are *observed as decreased performance*
- Requires static analysis or *binary instrumentation* to measure AI

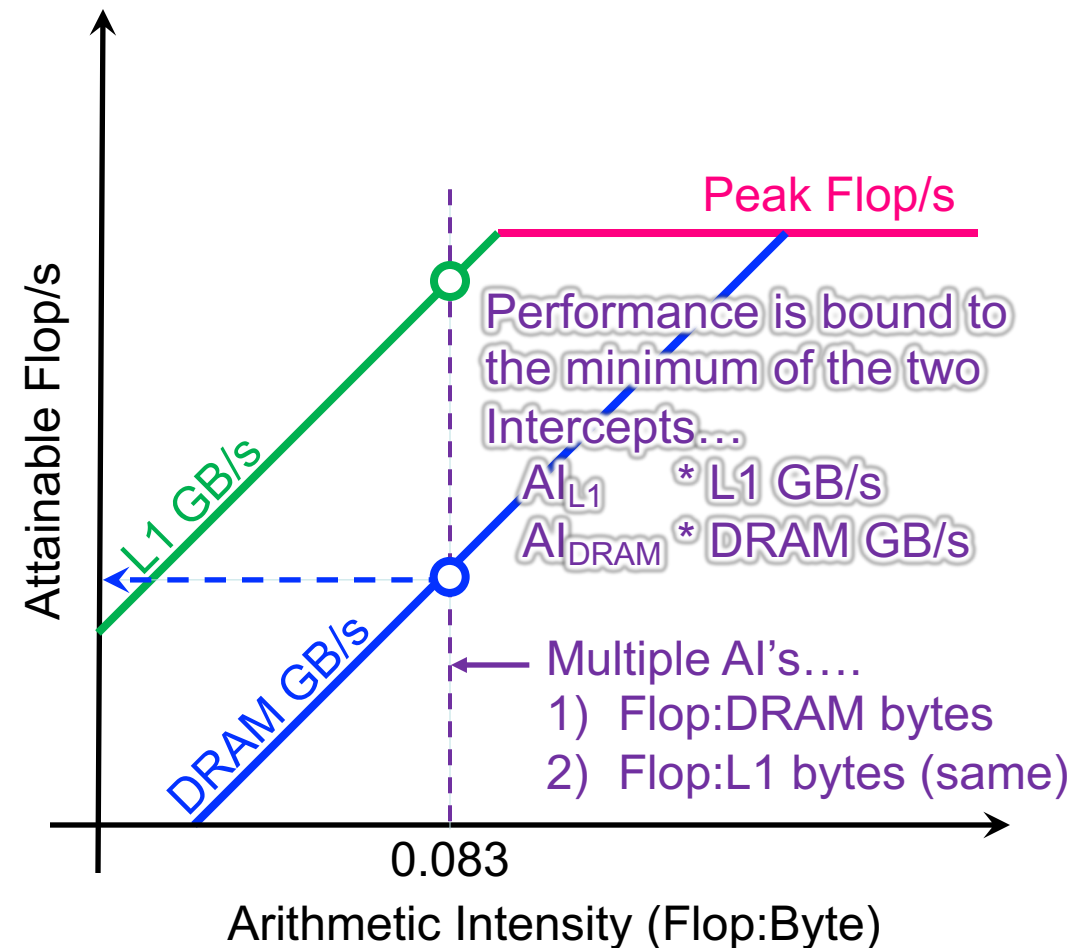
Example: STREAM

- L1 AI...
 - 2 flops
 - 2 x 8B load (old)
 - 1 x 8B store (new)
 - = 0.08 flops per byte
- No cache reuse...
 - Iteration i doesn't touch any data associated with iteration $i + \text{delta}$ for any delta .
- ... leads to a DRAM AI equal to the L1 AI

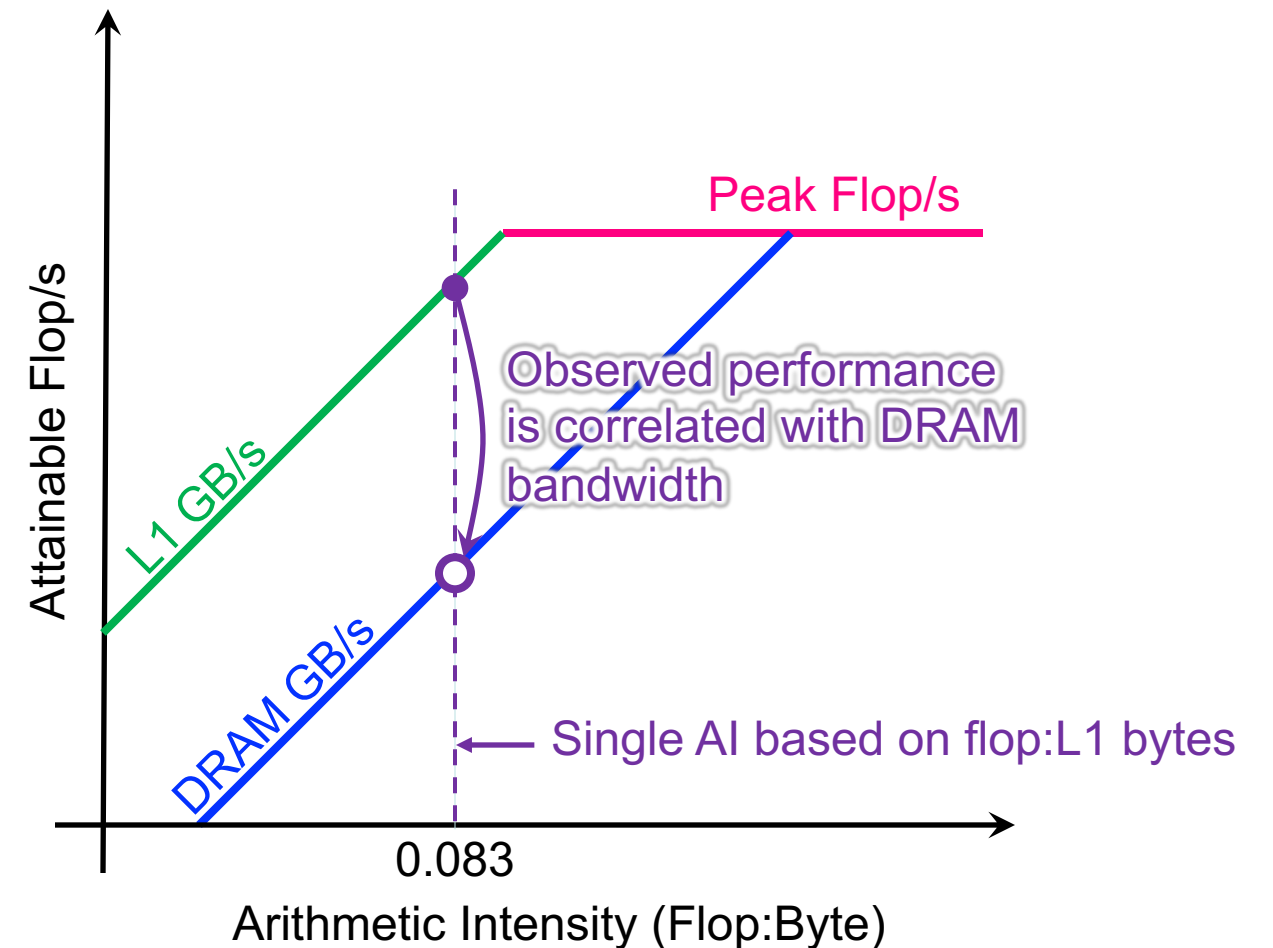
```
#pragma omp parallel for  
for(i=0;i<N;i++){  
    z[i] = x[i] + alpha*y[i];  
}
```


Example: STREAM

Hierarchical Roofline



Cache-Aware Roofline



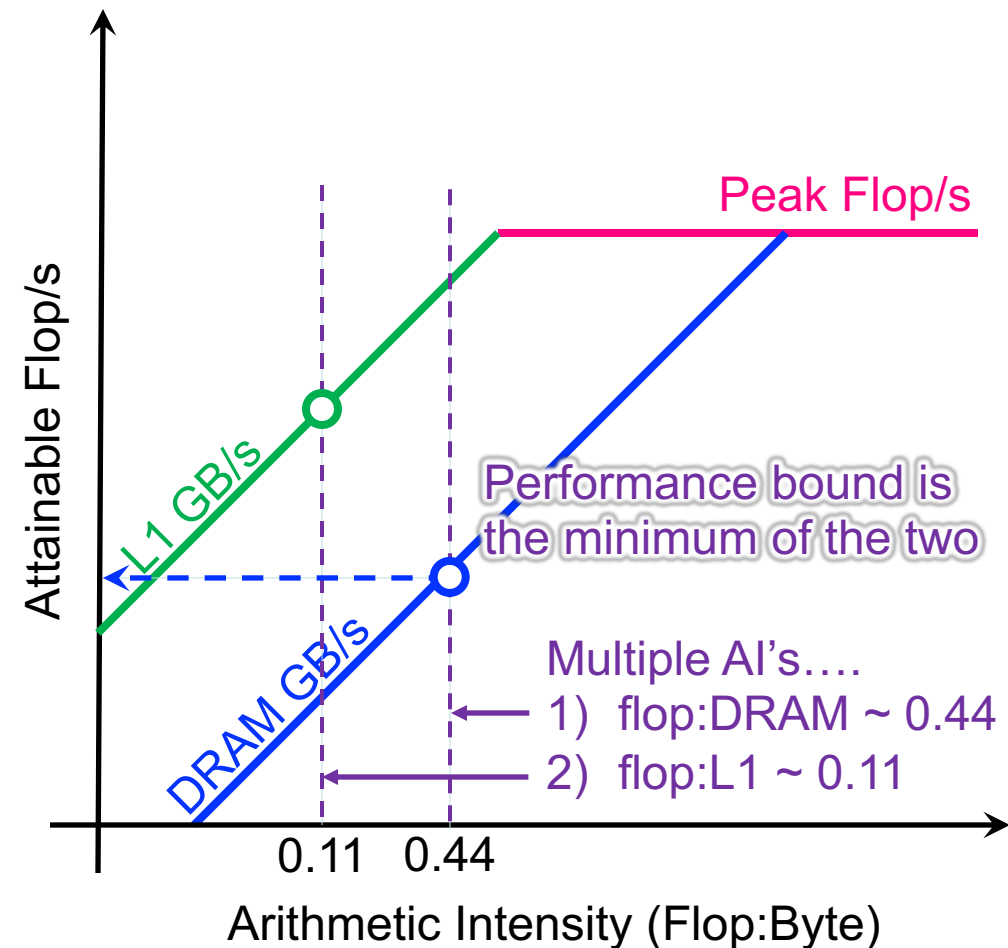
Example: 7-point Stencil (Small Problem)

- L1 AI...
 - 7 flops
 - 7 x 8B load (old)
 - 1 x 8B store (new)
 - = 0.11 flops per byte
 - some compilers may do register shuffles to reduce the number of loads.
- Moderate cache reuse...
 - `old[k][j][i+1]` is reused on next iteration of `i`.
 - `old[k][j+1][i]` is reused on next iteration of `j`.
 - `old[k+1][j][i]` is reused on next iterations of `k`.
- ... leads to DRAM AI larger than the L1 AI

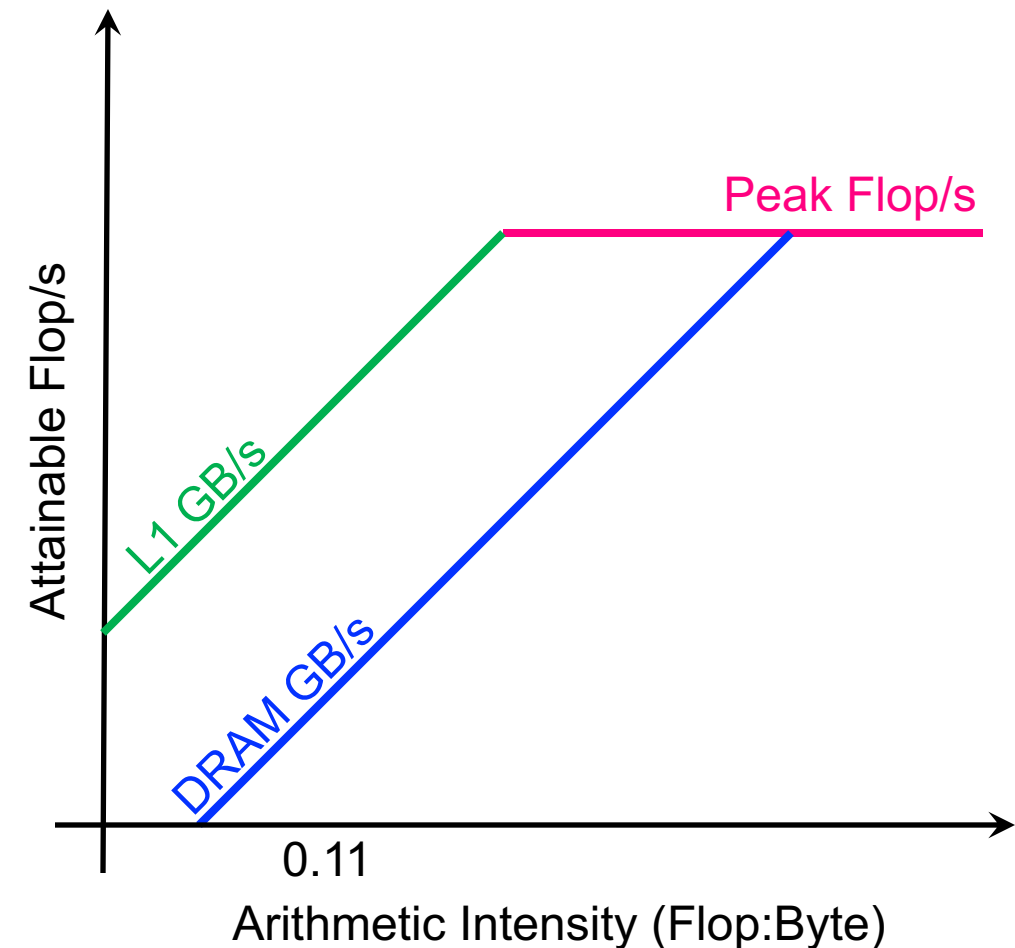
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for(k=1;k<dim+1;k++){
for(j=1;j<dim+1;j++){
for(i=1;i<dim+1;i++){
    new[k][j][i] = -6.0*old[k][j][i]
                  + old[k][j][i-1]
                  + old[k][j][i+1]
                  + old[k][j-1][i]
                  + old[k][j+1][i]
                  + old[k-1][j][i]
                  + old[k+1][j][i];
}}}
}
```

Example: 7-point Stencil (Small Problem)

Hierarchical Roofline

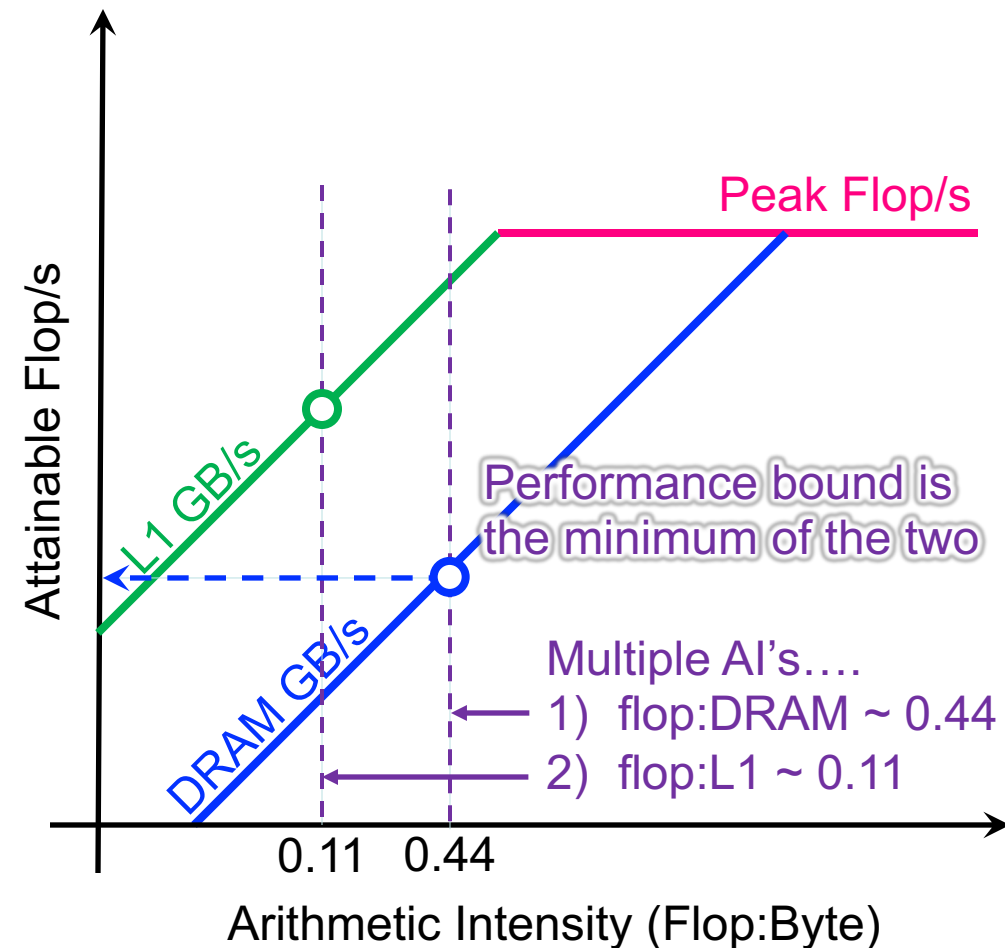


Cache-Aware Roofline

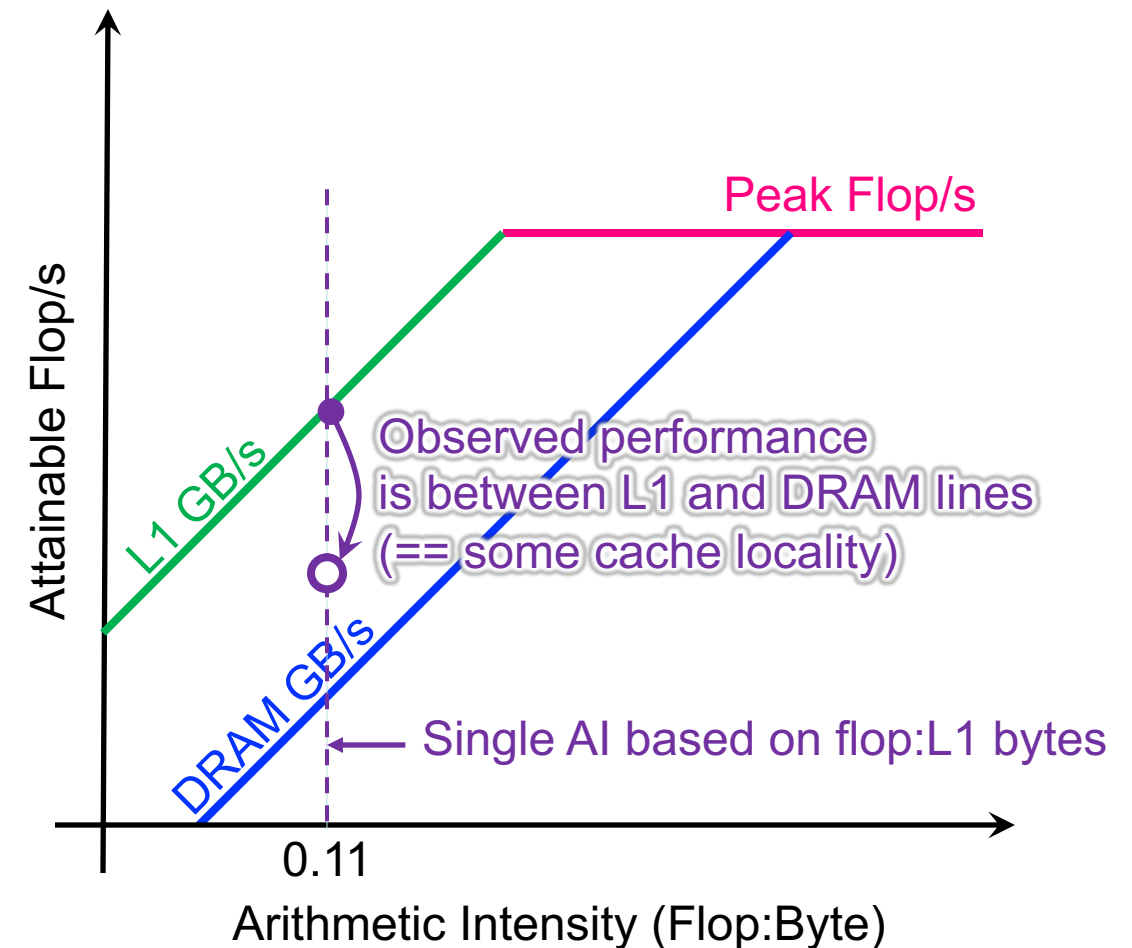


Example: 7-point Stencil (Small Problem)

Hierarchical Roofline

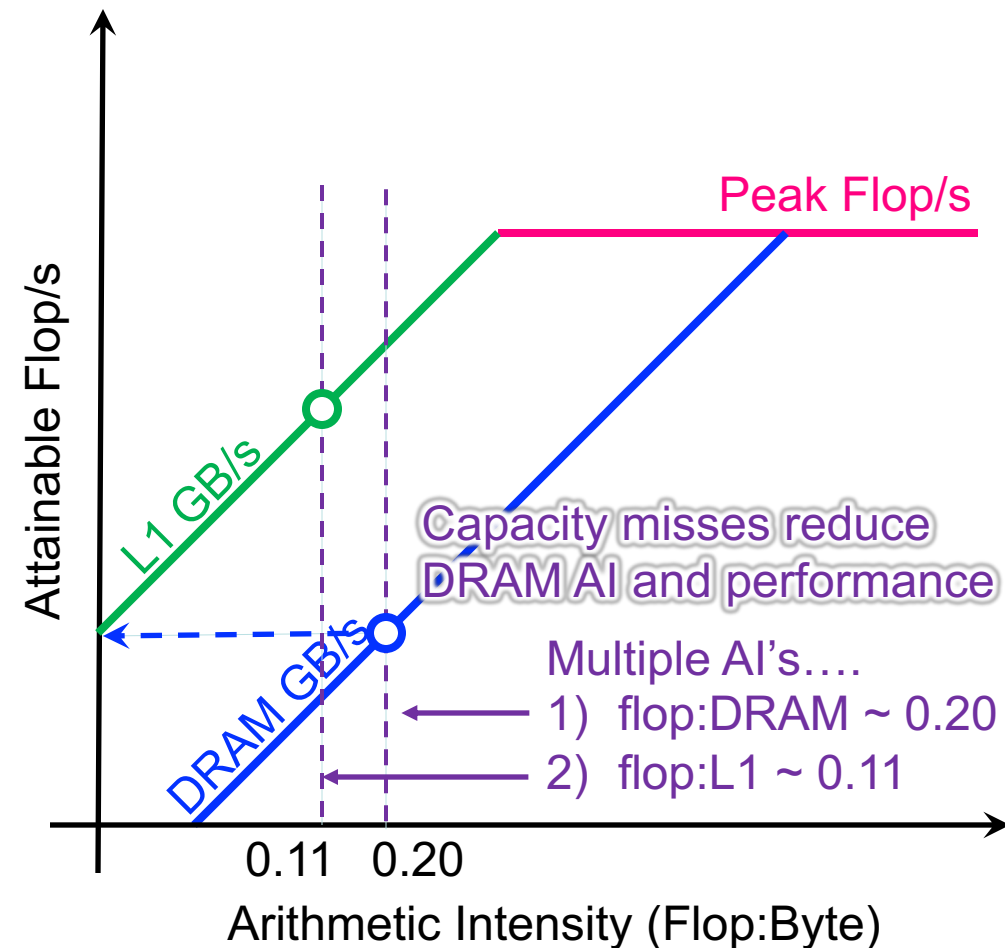


Cache-Aware Roofline

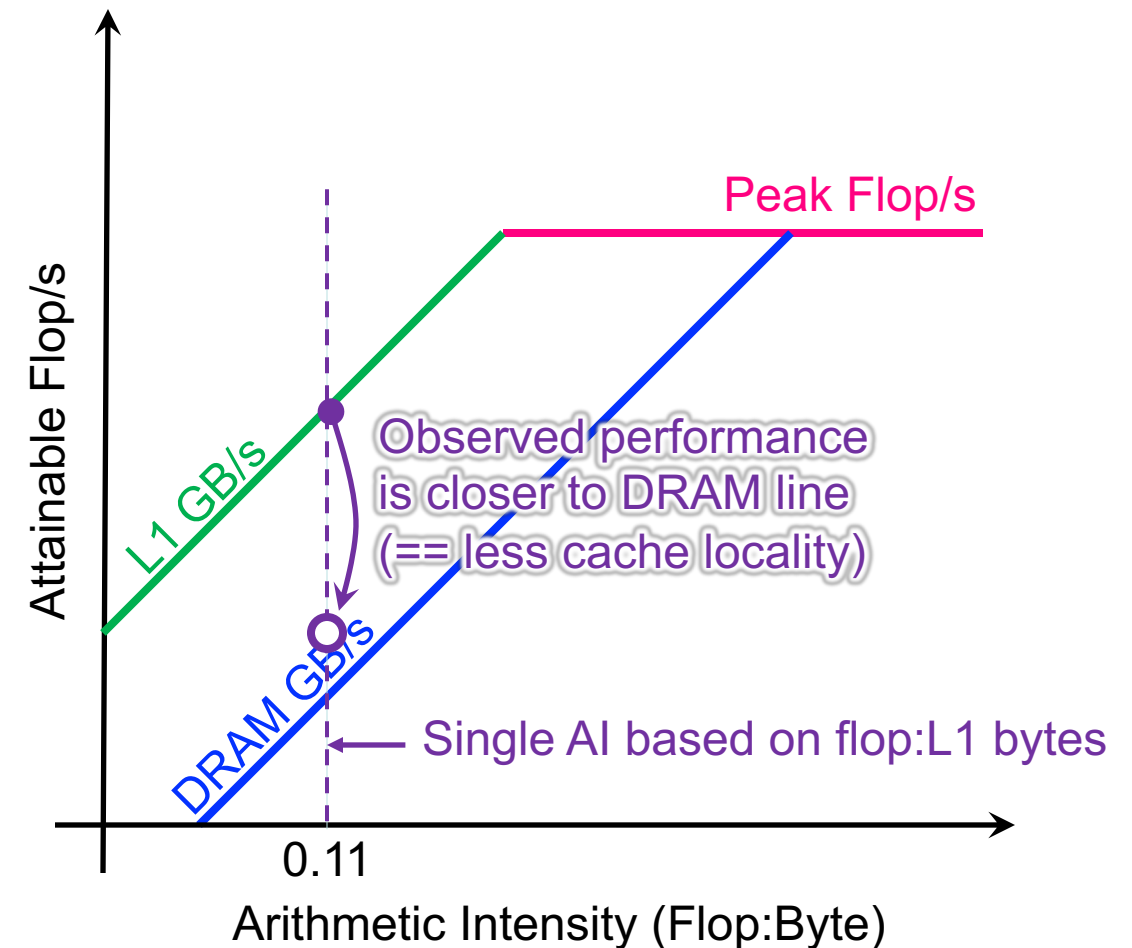


Example: 7-point Stencil (Large Problem)

Hierarchical Roofline

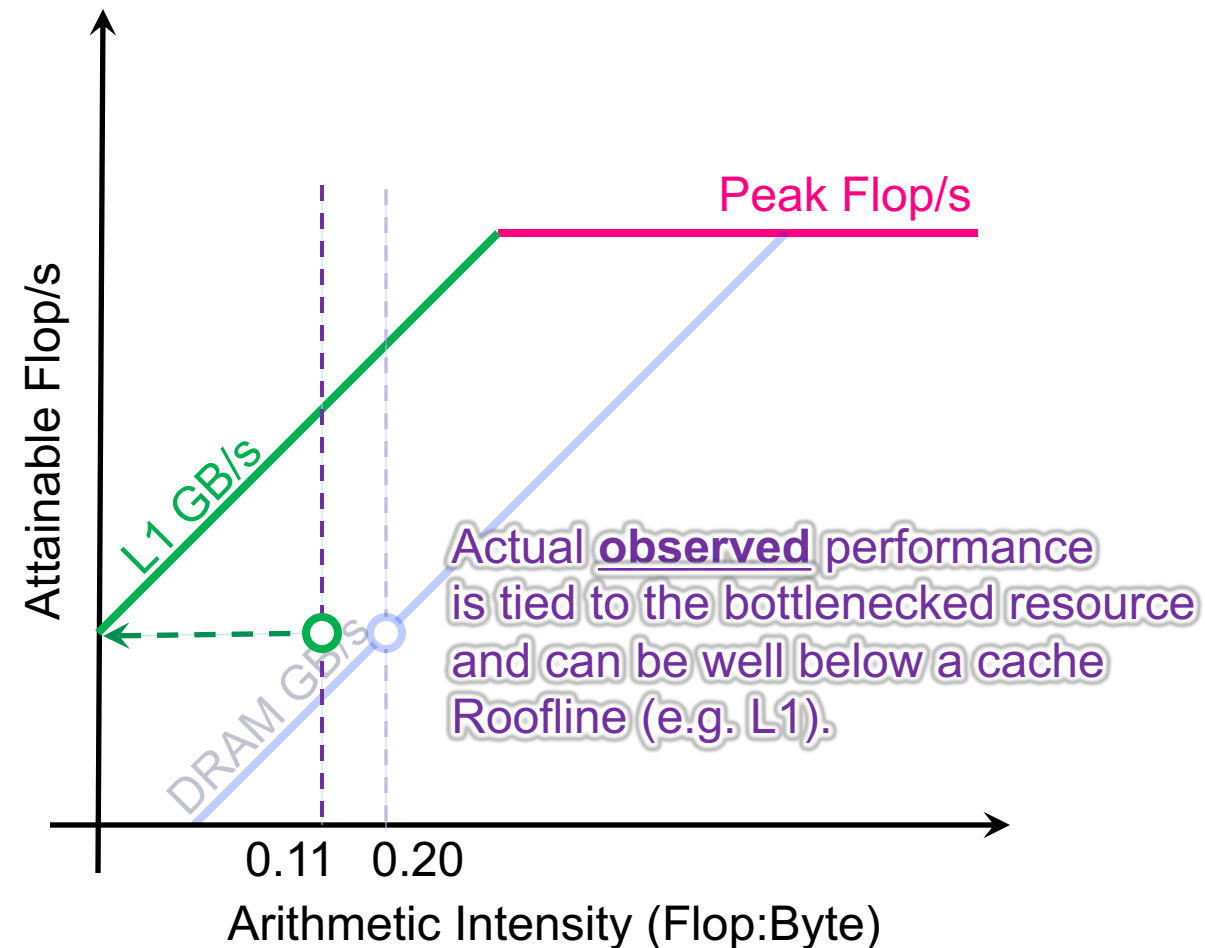


Cache-Aware Roofline

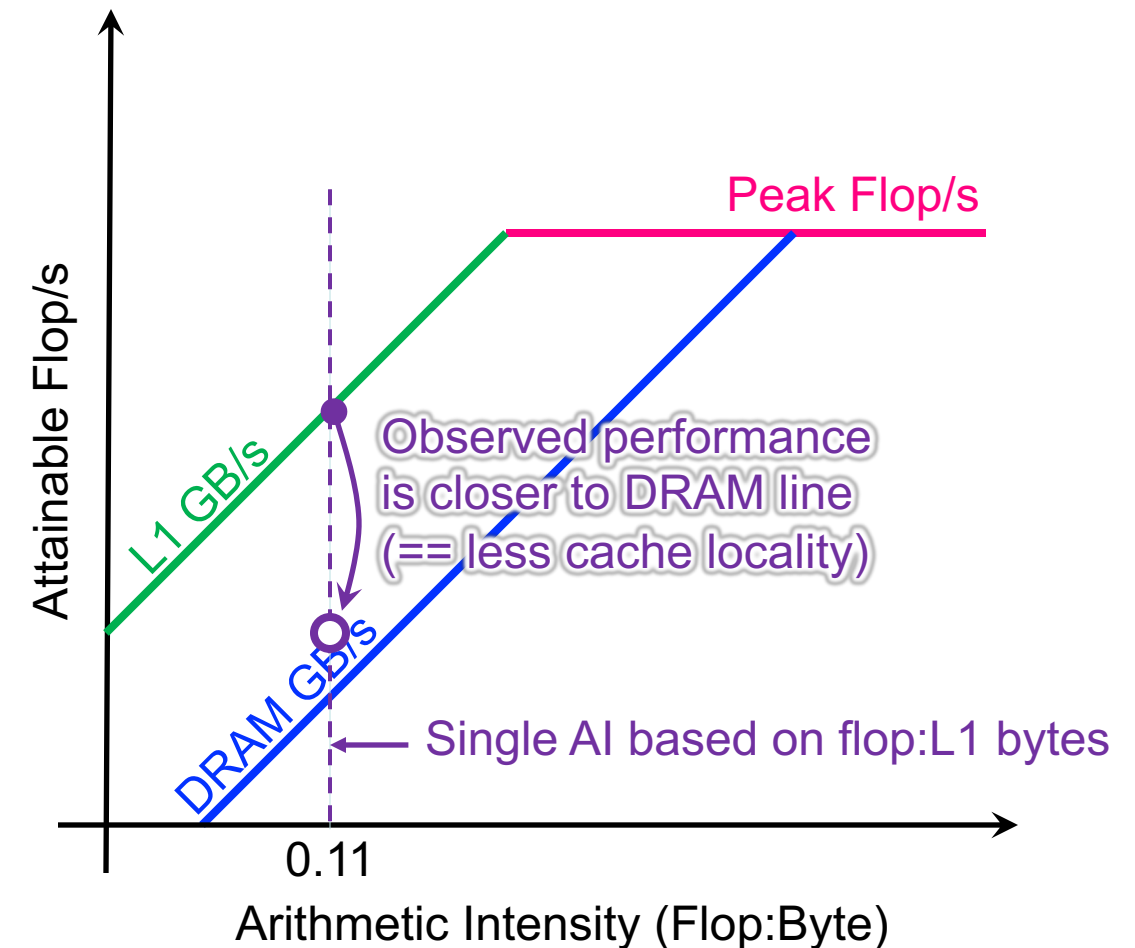


Example: 7-point Stencil (Observed Perf.)

Hierarchical Roofline

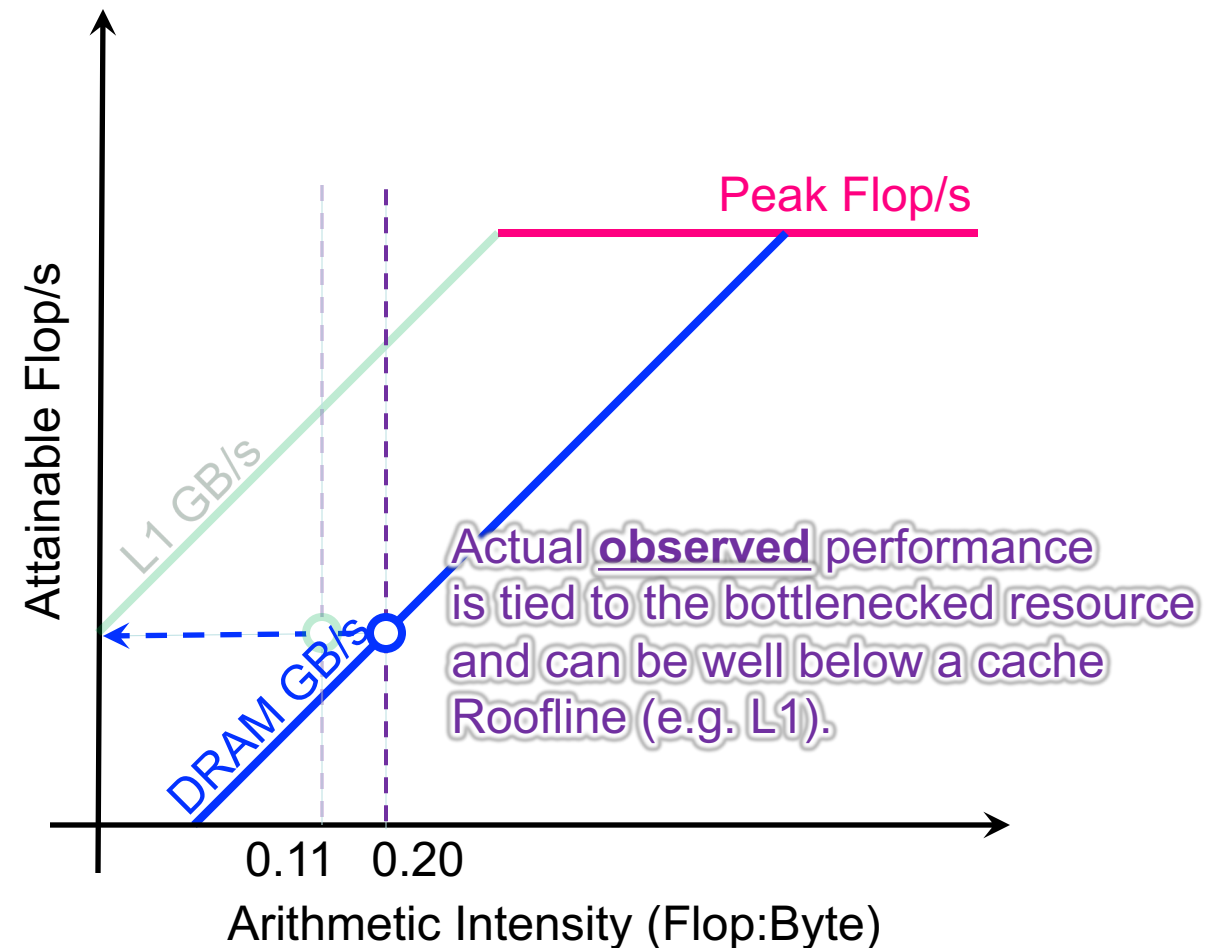


Cache-Aware Roofline

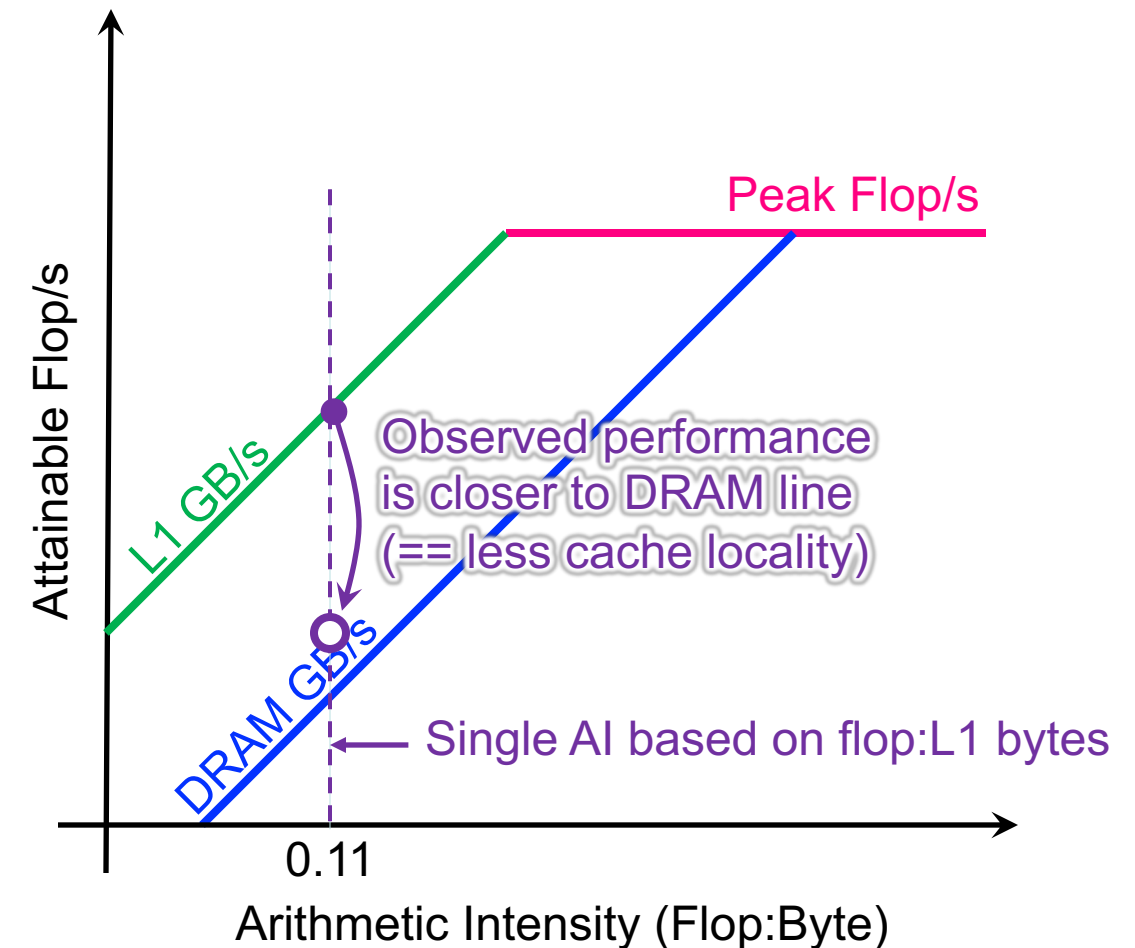


Example: 7-point Stencil (Observed Perf.)

Hierarchical Roofline



Cache-Aware Roofline



Questions?

Don't forget to take the Survey...

<http://bit.ly/sc18-eval>





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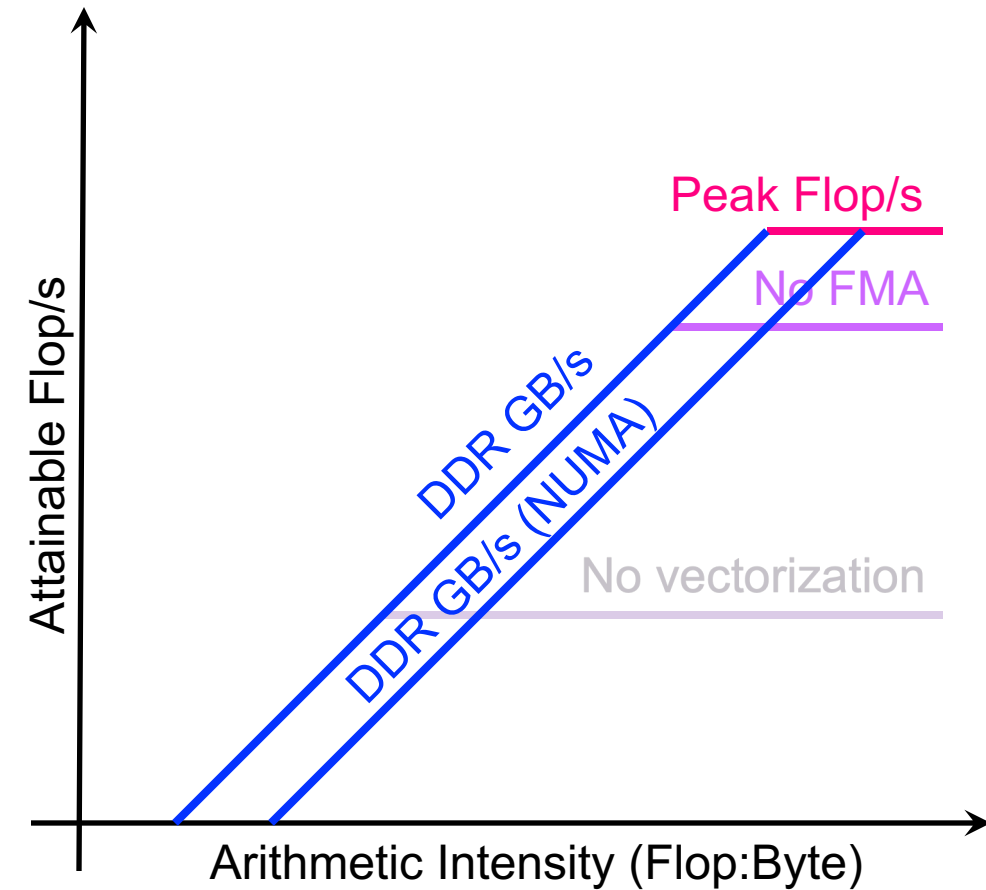
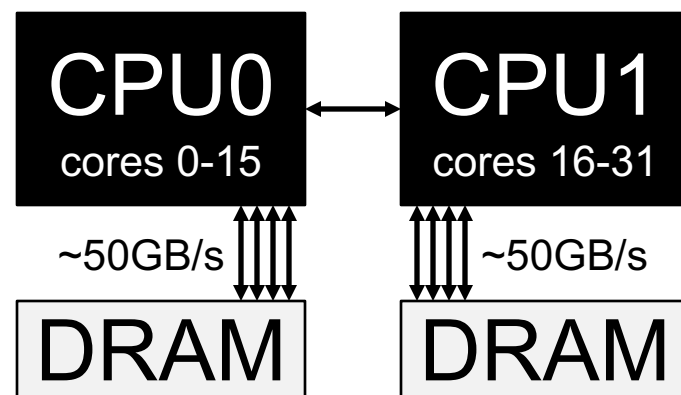
U.S. DEPARTMENT OF
ENERGY

Backup

Refining Roofline: NUMA

NUMA Effects

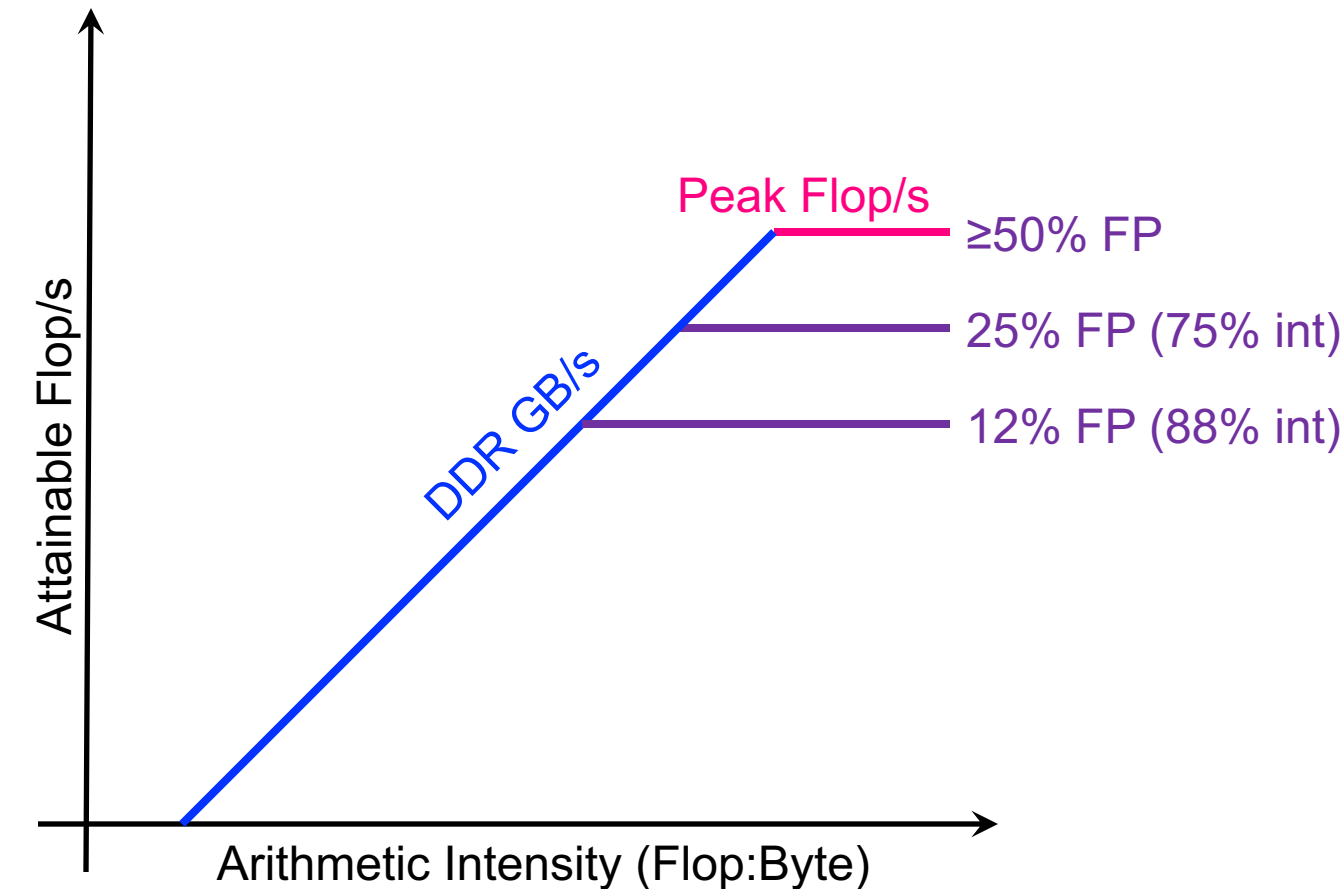
- Cori's Haswell nodes are built from 2 Xeon processors (sockets)
 - Memory attached to each socket (fast)
 - Interconnect that allows remote memory access (slow == NUMA)
 - Improper memory allocation can result in more than a 2x performance penalty



Refining Roofline: Instruction Issue Bandwidth

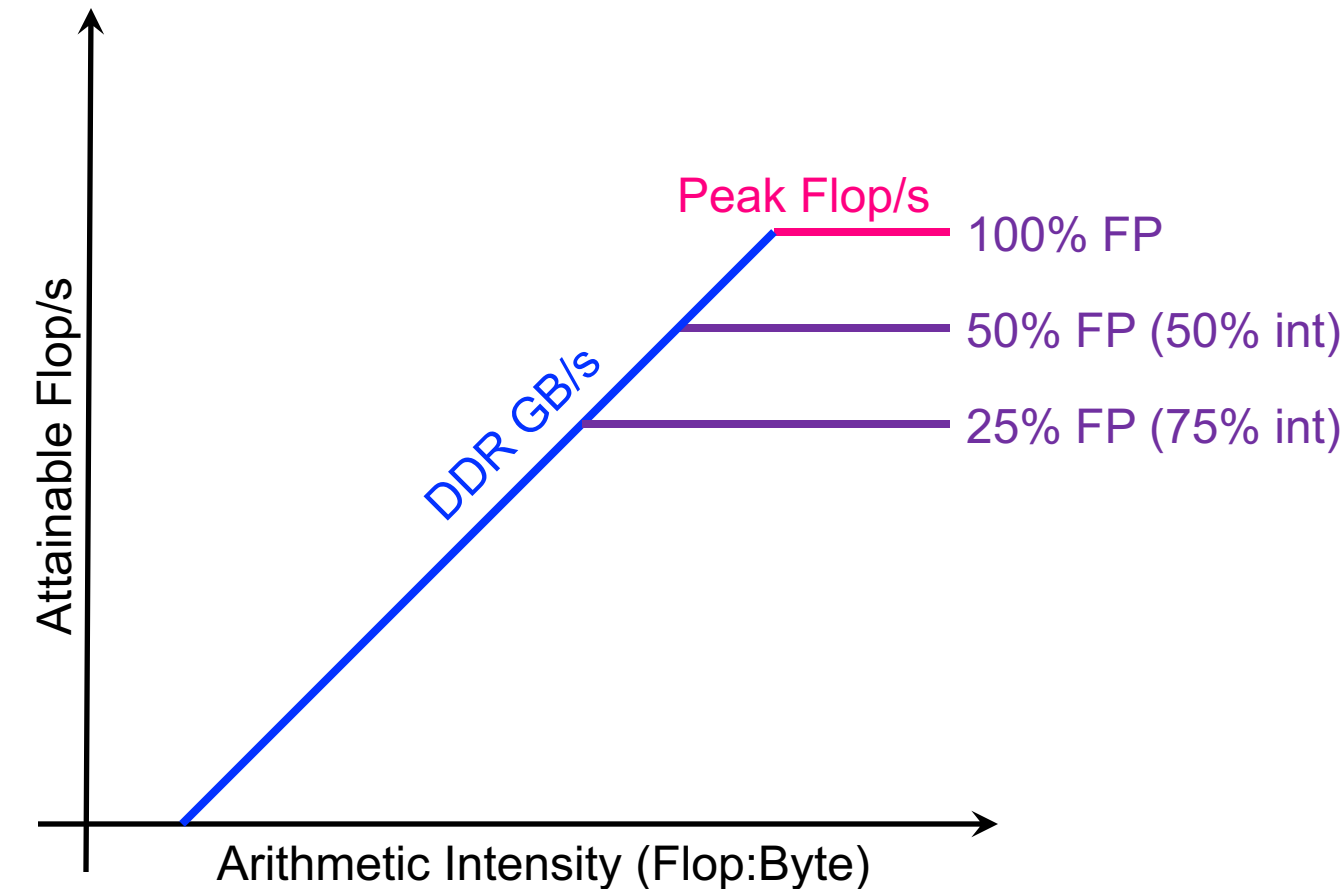
Superscalar vs. Instruction mix

- Define in-core ceilings based on instruction mix...
- e.g. Haswell
 - 4-issue superscalar
 - Only 2 FP data paths
 - Requires 50% of the instructions to be FP to get peak performance



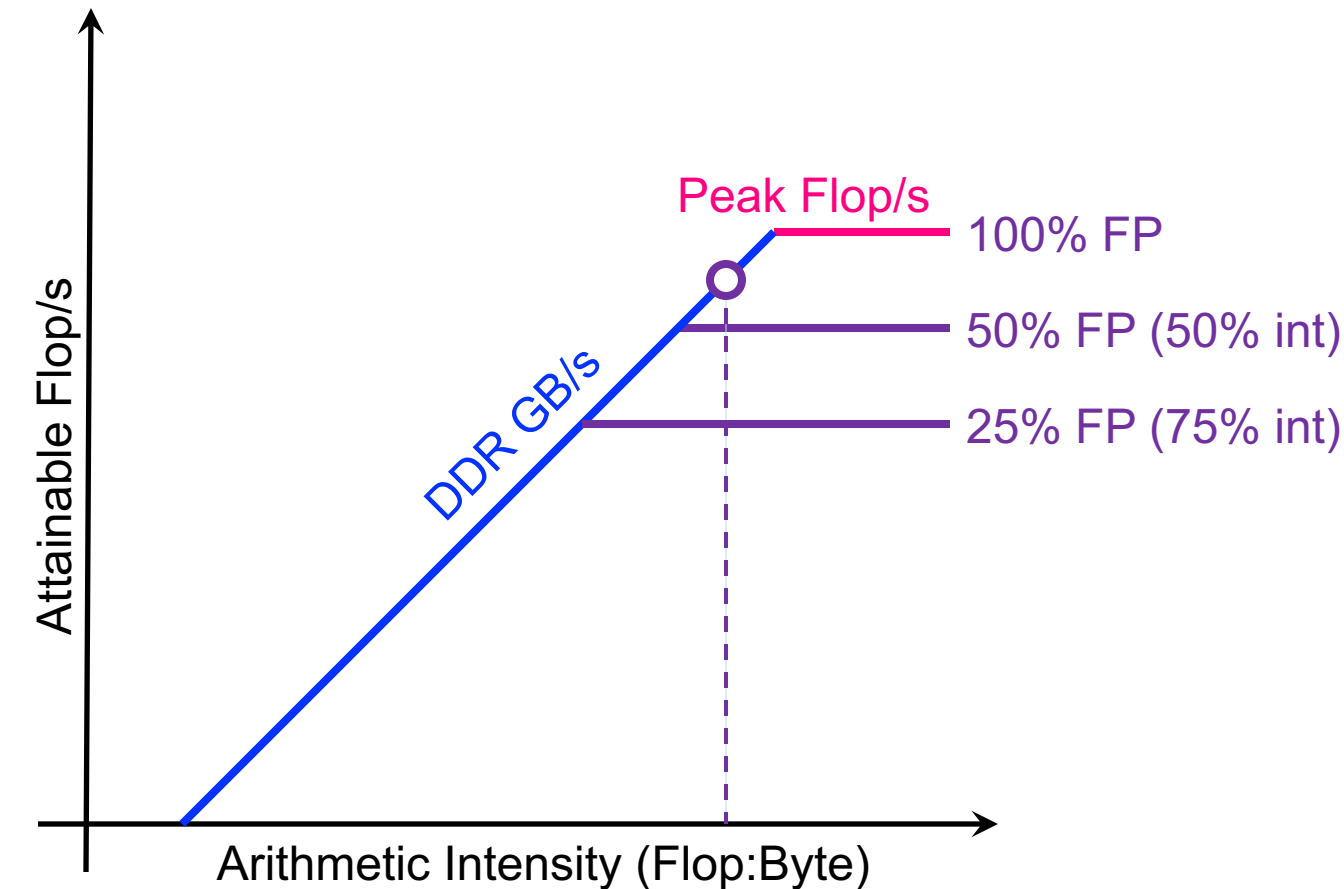
Superscalar vs. Instruction mix

- Define in-core ceilings based on instruction mix...
- e.g. Haswell
 - 4-issue superscalar
 - Only 2 FP data paths
 - Requires 50% of the instructions to be FP to get peak performance
- e.g. KNL
 - 2-issue superscalar
 - 2 FP data paths
 - Requires 100% of the instructions to be FP to get peak performance



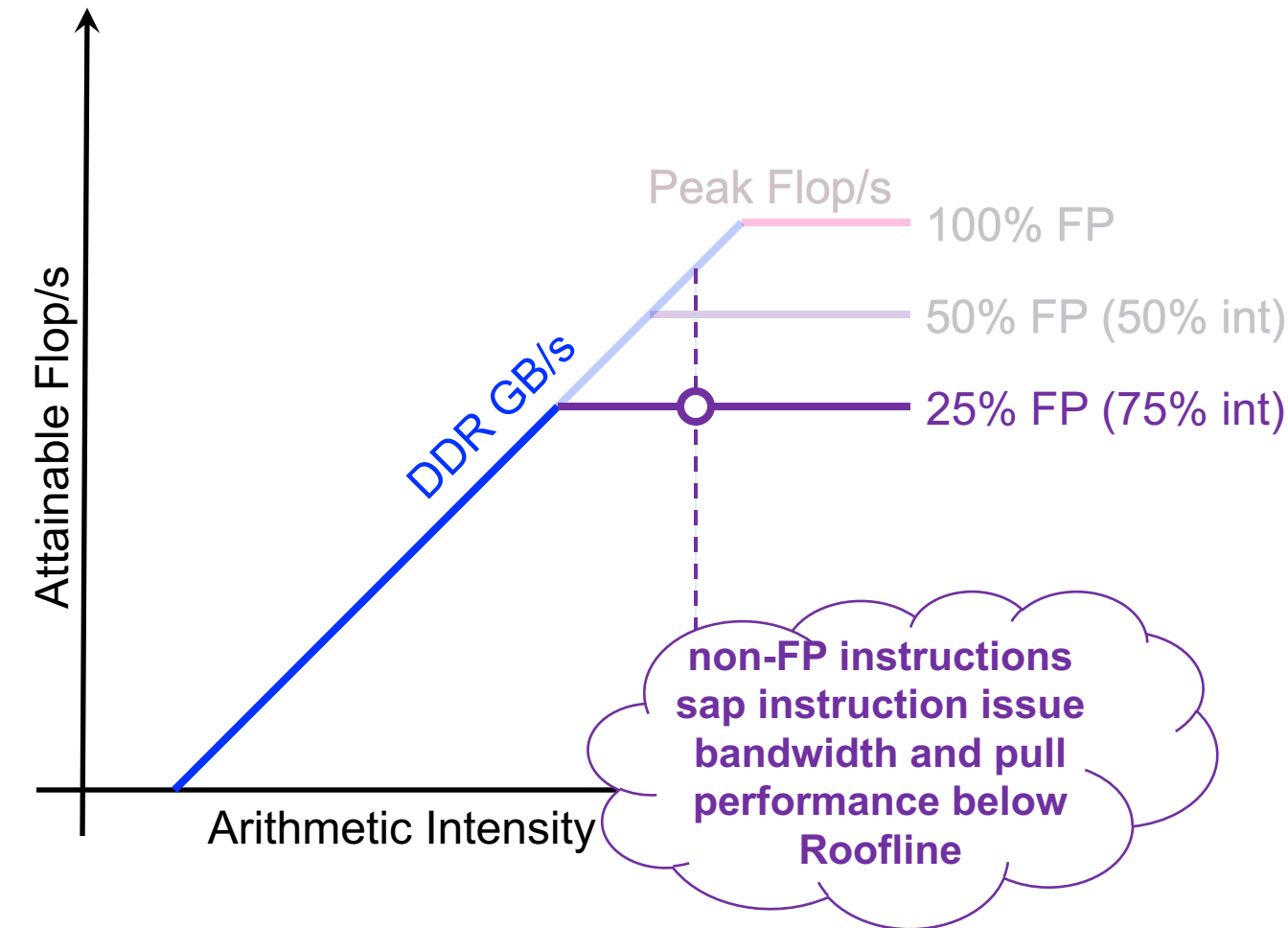
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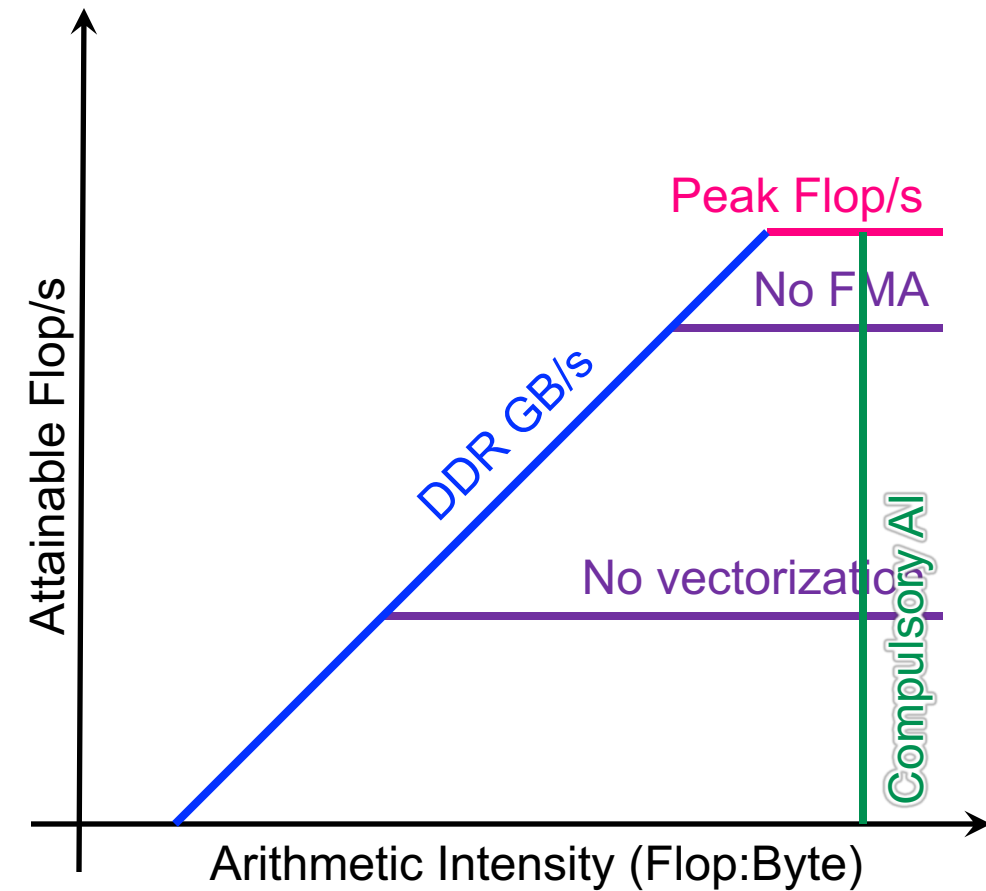
Refining Roofline:

Compulsory, Capacity, and Conflict misses

Locality Walls

- Naively, we can bound AI using only compulsory cache misses

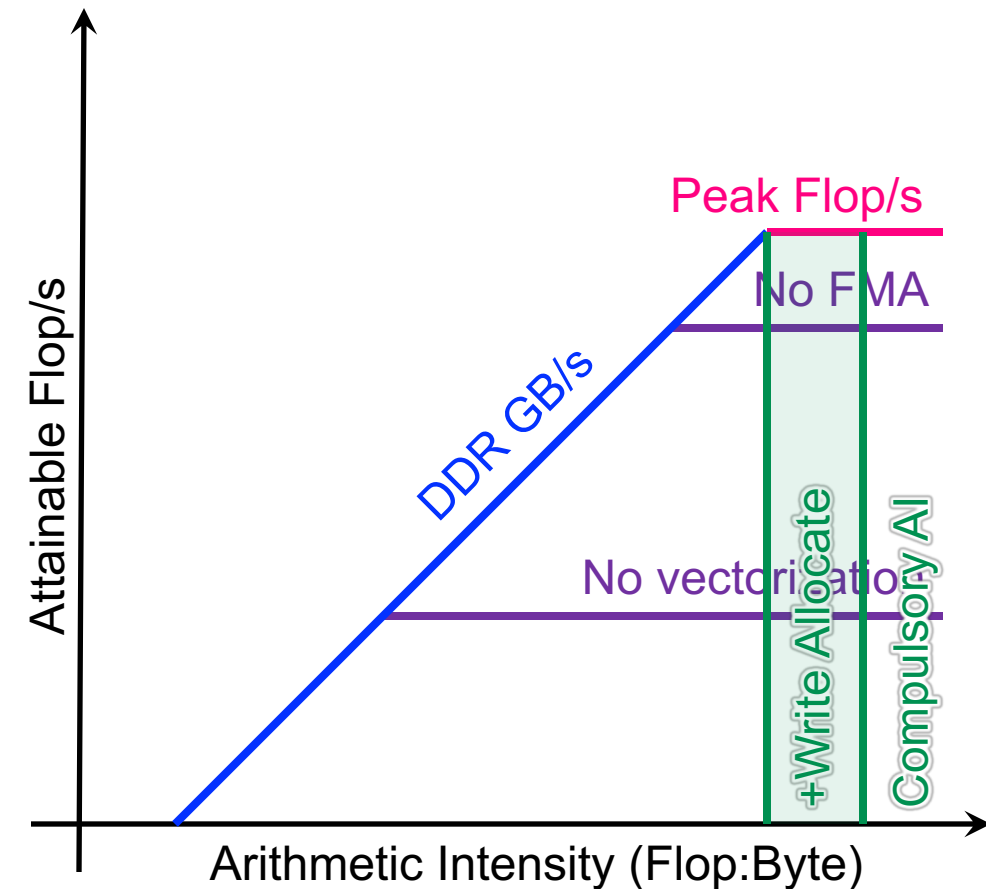
$$AI = \frac{\text{\#Flop's}}{\text{Compulsory Misses}}$$



Locality Walls

- Naively, we can bound AI using only compulsory cache misses
- However, write allocate caches can lower AI

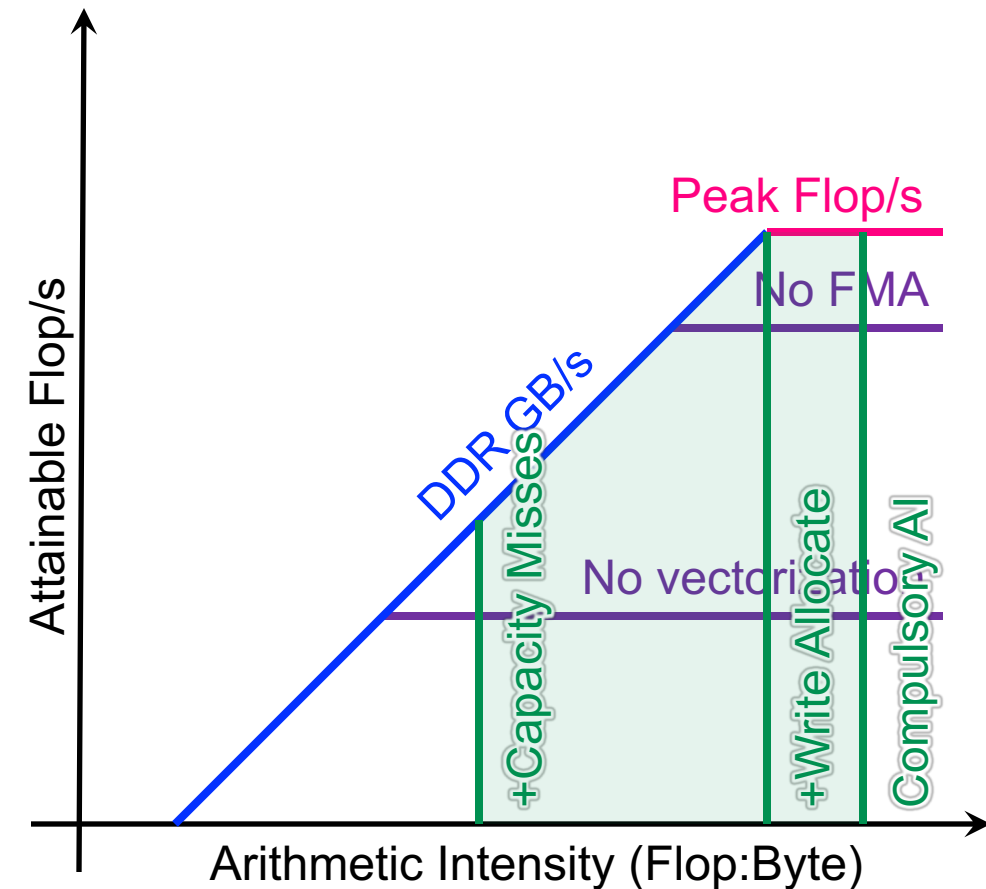
$$AI = \frac{\text{\#Flop's}}{\text{Compulsory Misses} + \text{Write Allocates}}$$



Locality Walls

- Naively, we can bound AI using only compulsory cache misses
- However, write allocate caches can lower AI
- Cache capacity misses can have a huge penalty

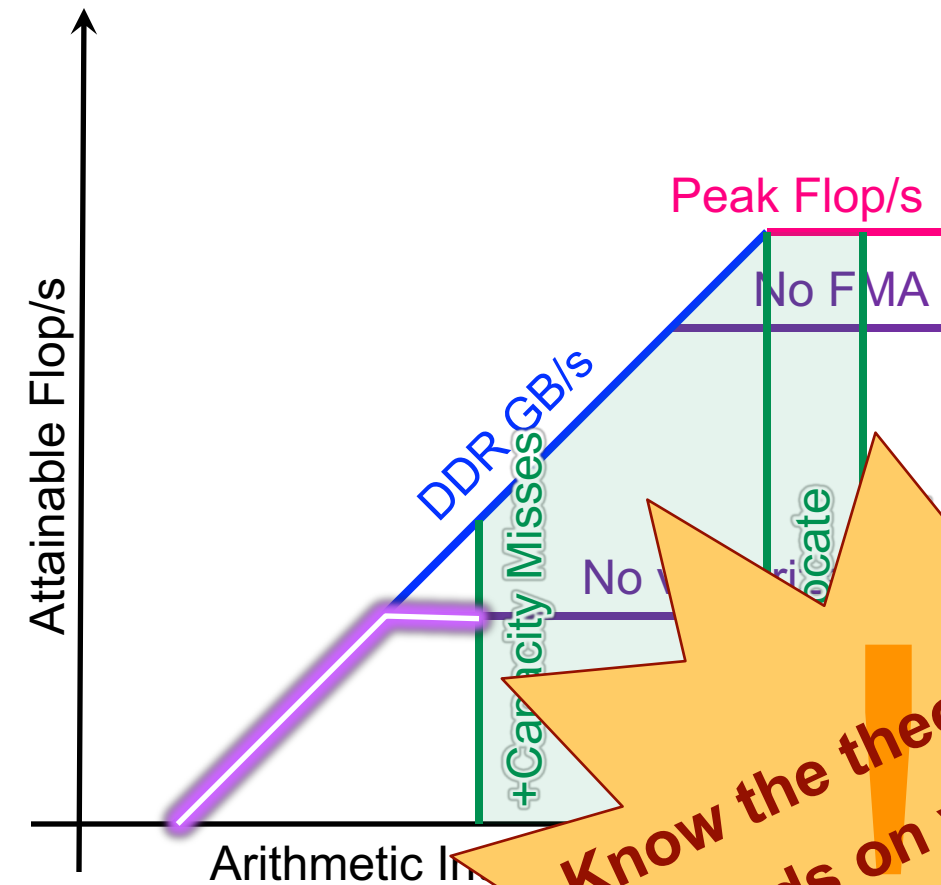
$$AI = \frac{\text{\#Flop's}}{\text{Compulsory Misses} + \text{Write Allocates} + \text{Capacity Misses}}$$



Locality Walls

- Naively, we can bound AI using only compulsory cache misses
 - However, write allocate caches can lower AI
 - Cache capacity misses can have a huge penalty
- **Compute bound became memory bound**

$$AI = \frac{\text{\#Flop's}}{\text{Compulsory Misses} + \text{Write Allocates} + \text{Capacity Misses}}$$





LIKWID:

Performance Counters

LIKWID

- LIKWID provides easy to use wrappers for measuring performance counters...
 - ✓ **Works on NERSC production systems**
 - ✓ Distills counters into user-friendly metrics (e.g. MCDRAM Bandwidth)
 - ✓ Minimal overhead (<1%)
 - ✓ Scalable in distributed memory (MPI-friendly)
 - ✓ Fast, high-level characterization
 - ✗ No timing breakdowns
 - ✗ Suffers from Garbage-in/Garbage Out
(i.e. hardware counter must be sufficient and correct)

<https://github.com/RRZE-HPC/likwid>

<http://www.nersc.gov/users/software/performance-and-debugging-tools/likwid>