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, Oliker, 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.

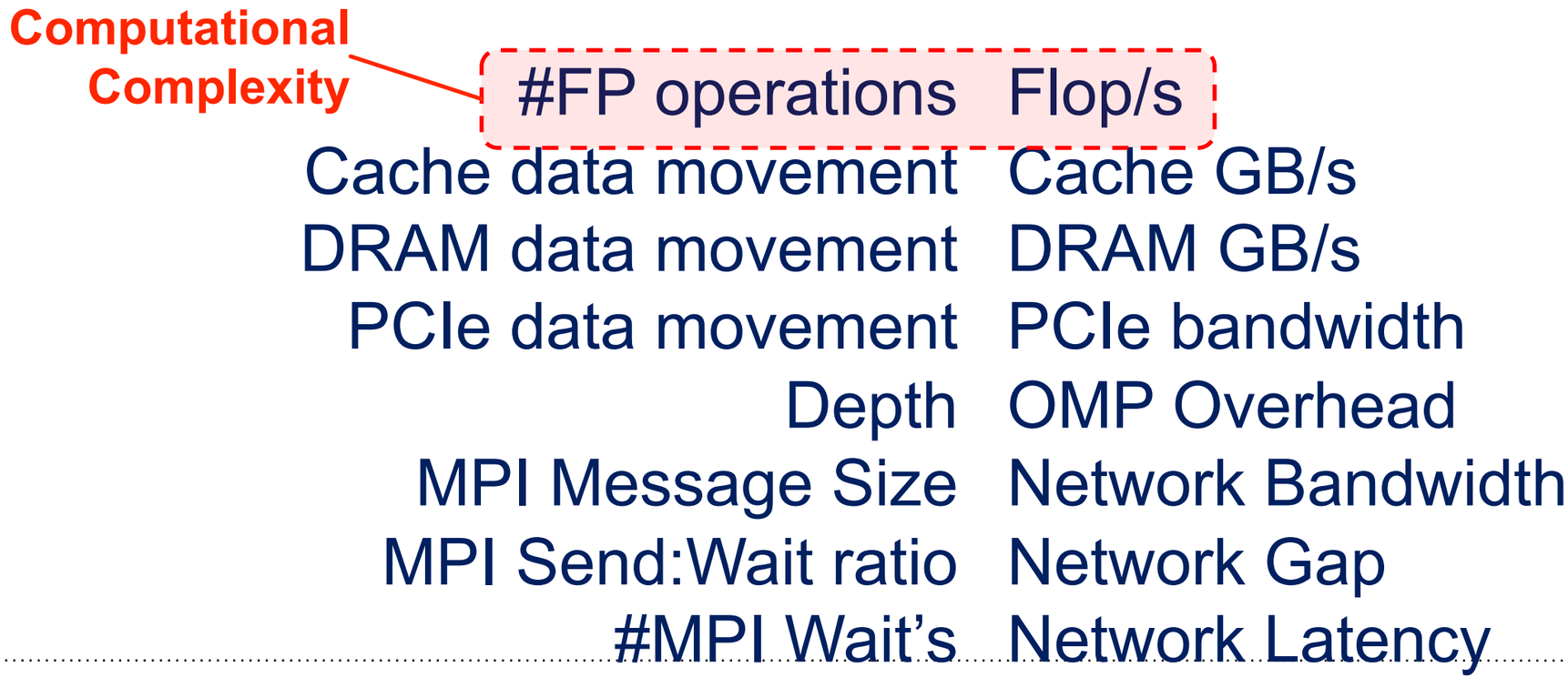
Performance Models

- 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…



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Culler, et al, "LogP: a practical model of parallel computation", CACM, 1996.

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

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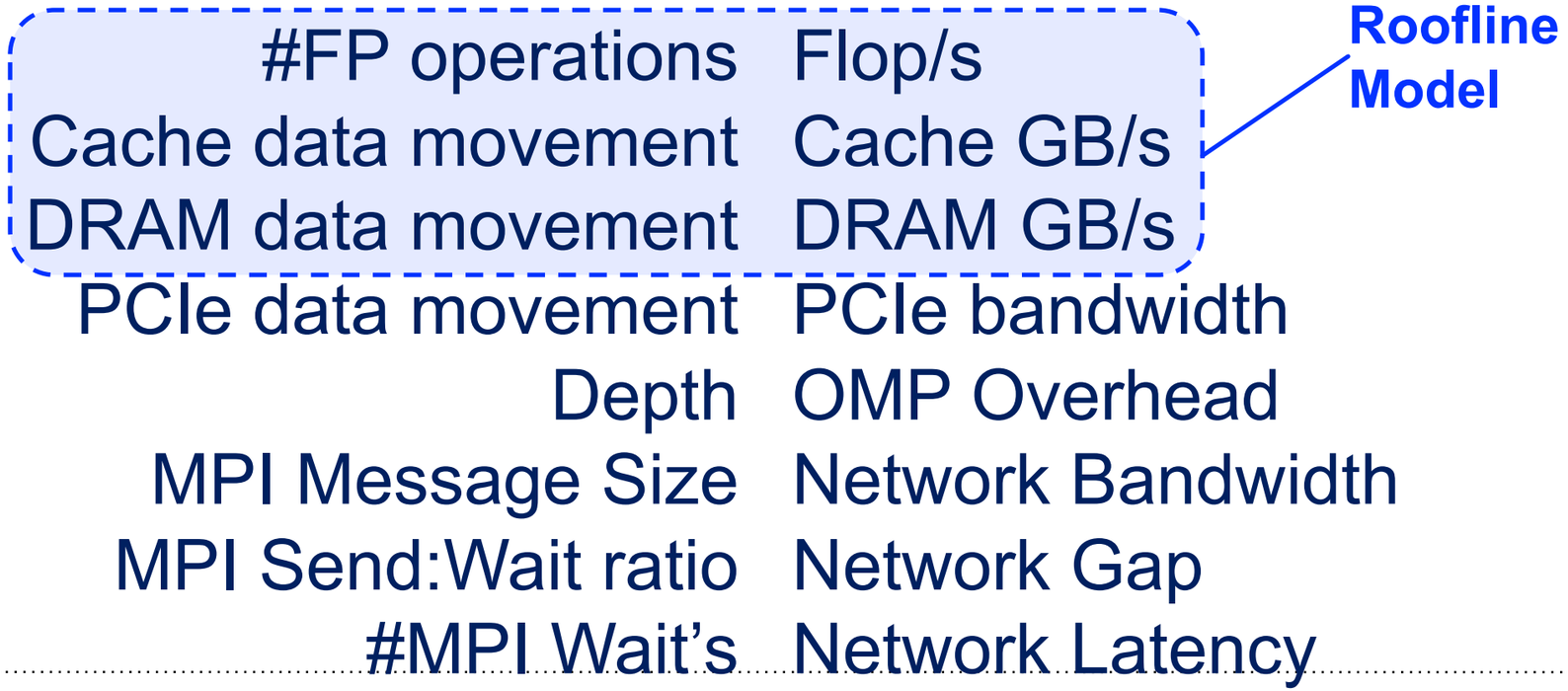


Williams et al, "Roofline: An Insightful Visual Performance Model For Multicore Architectures", CACM, 2009.

Roofline Model:

Arithmetic Intensity and Bandwidth

Performance Models / Simulators

- Historically, many performance models and simulators tracked time to predict performance (i.e. counting cycles)

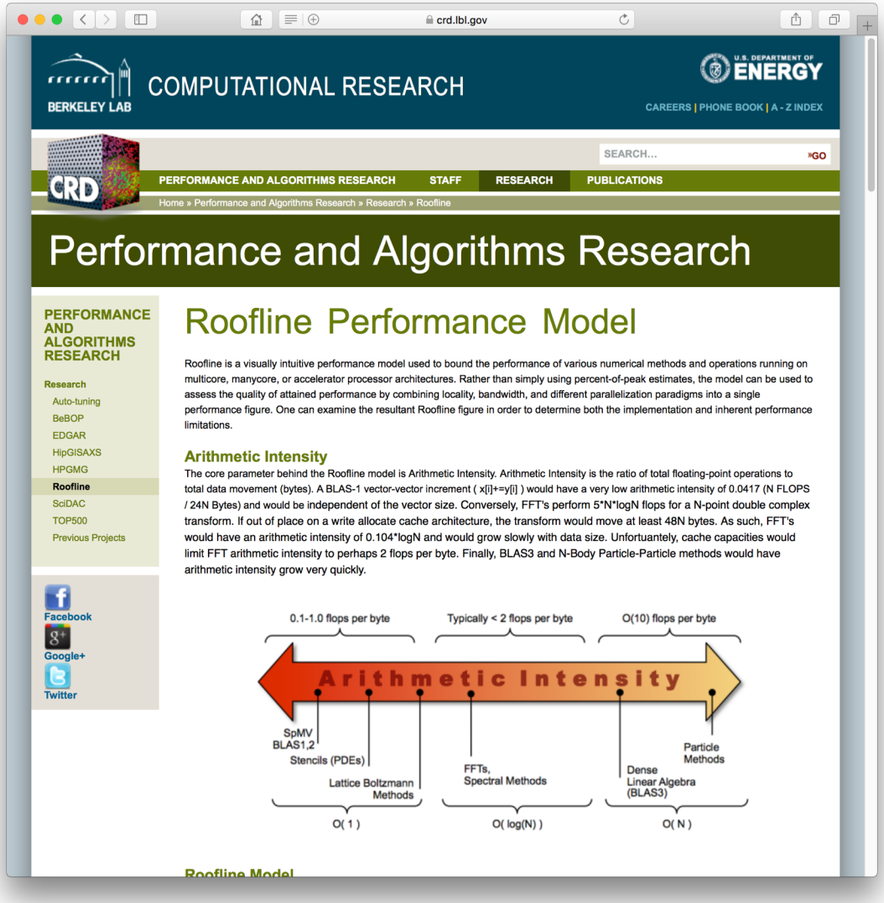
- The last two decades saw a number of latency-hiding techniques…
  - Out-of-order execution (hardware discovers parallelism to hide latency)
  - HW stream prefetching (hardware speculatively loads data)
  - Massive thread parallelism (independent threads satisfy the latency-bandwidth product)

- … 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 TPUs[1], etc…)

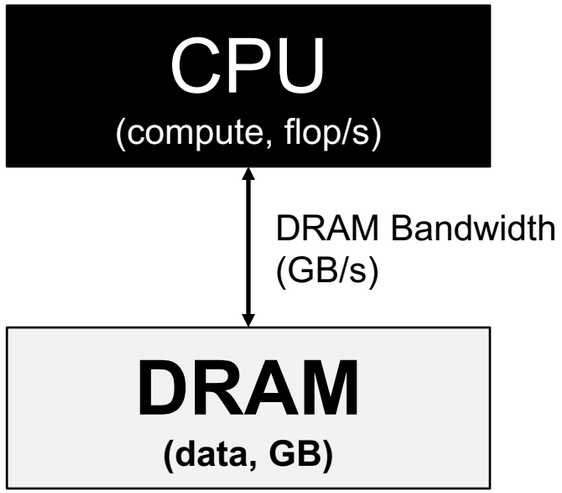


https://crd.lbl.gov/departments/computer-science/PAR/research/roofline

[1]Jouppi 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…



Time = max { #FP ops / Peak GFlop/s ; #Bytes / Peak GB/s }

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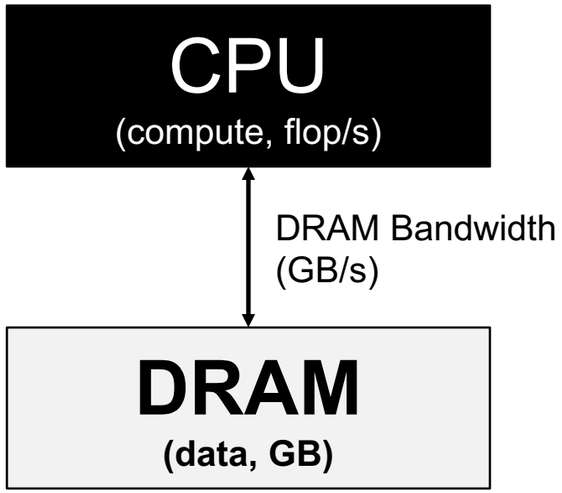

$$\frac{\text{Time}}{\#\text{FP ops}} = \max \begin{cases} 1 \,/\, \text{Peak GFlop/s} \\ \#\text{Bytes} \,/\, \#\text{FP ops} \,/\, \text{Peak GB/s} \end{cases}$$

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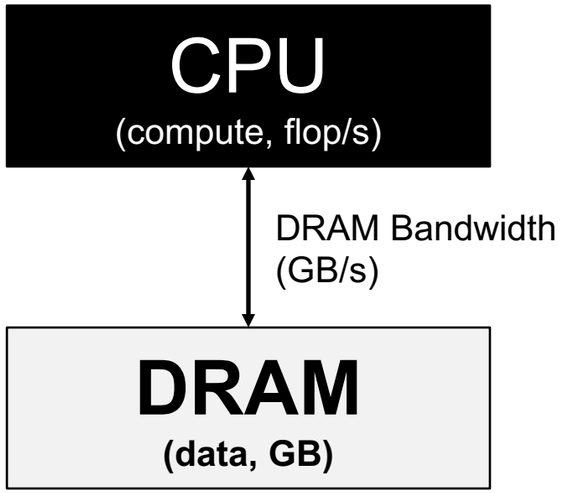

$$\frac{\#\text{FP ops}}{\text{Time}} = \min \begin{cases} \text{Peak GFlop/s} \\ (\#\text{FP ops} / \#\text{Bytes}) * \text{Peak GB/s} \end{cases}$$

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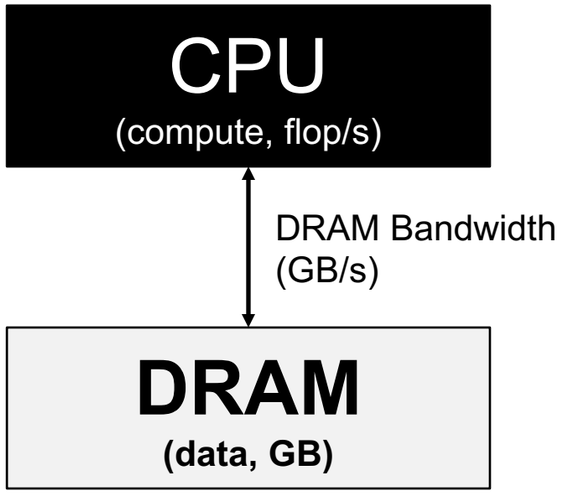
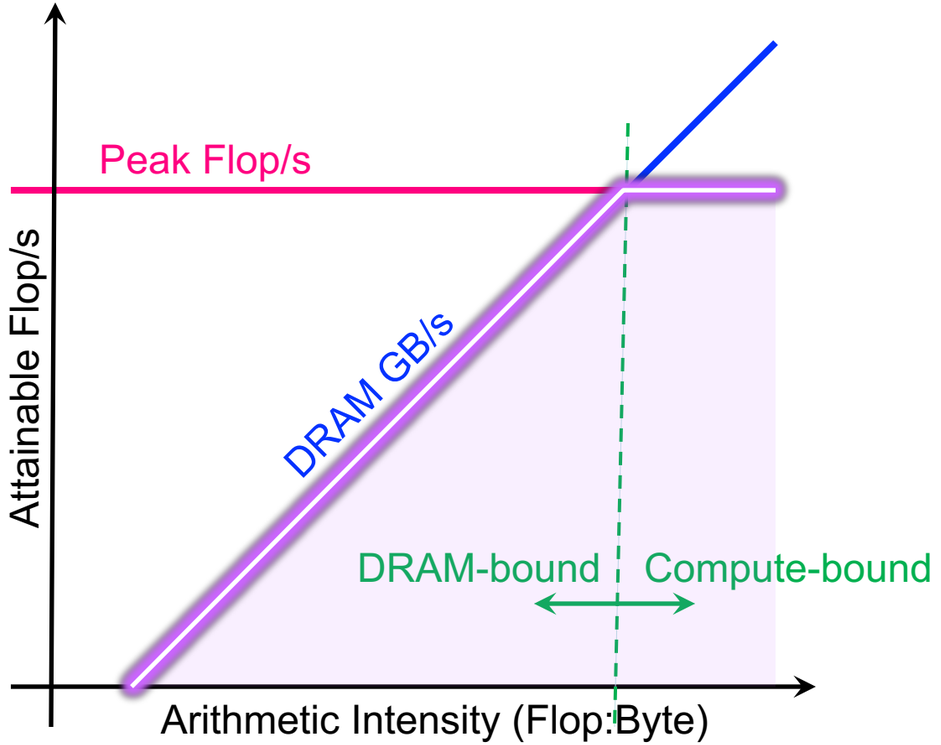


GFlop/s = min { Peak GFlop/s ; AI * Peak GB/s }

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…)



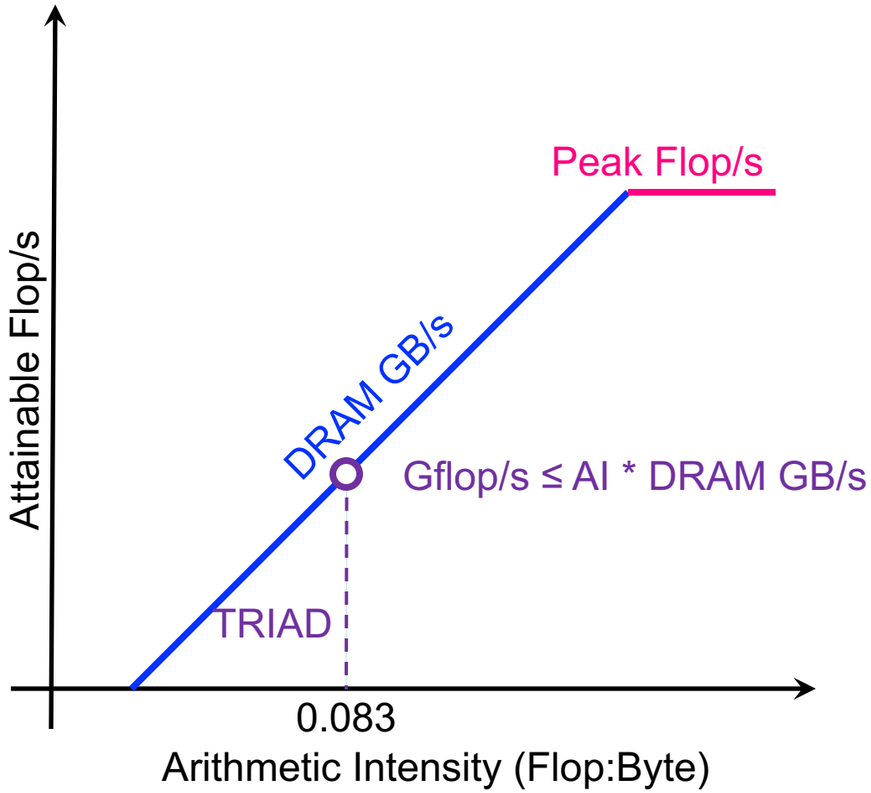
Roofline Example #1

- 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**

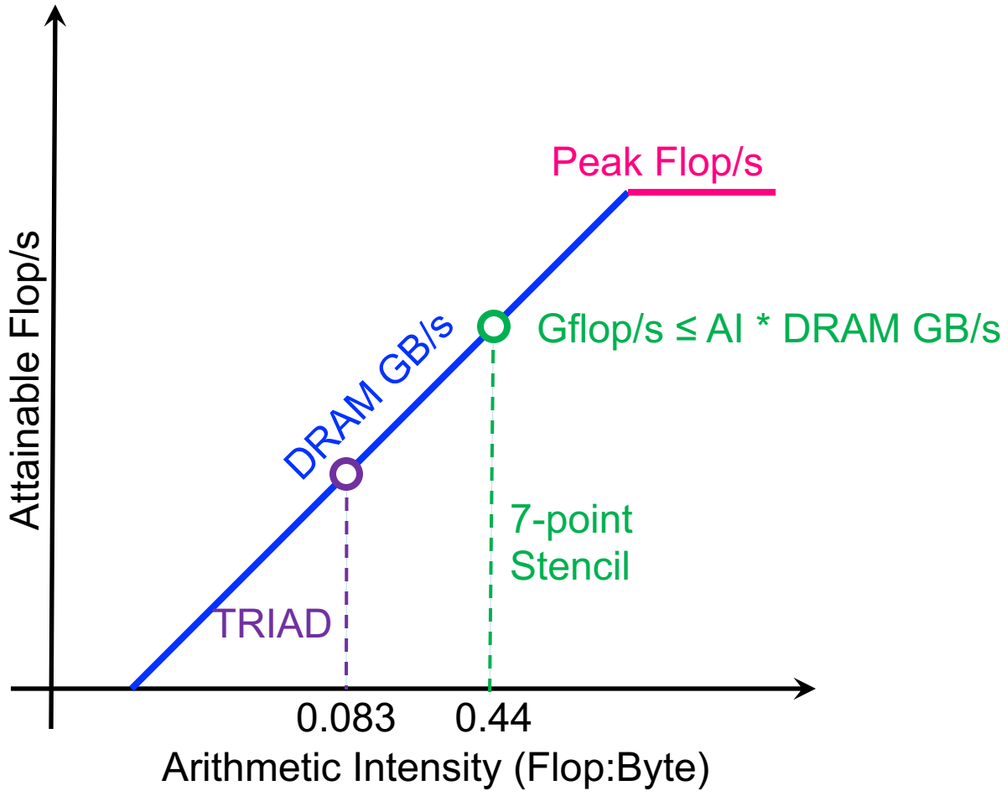


Roofline Example #2

- 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,**

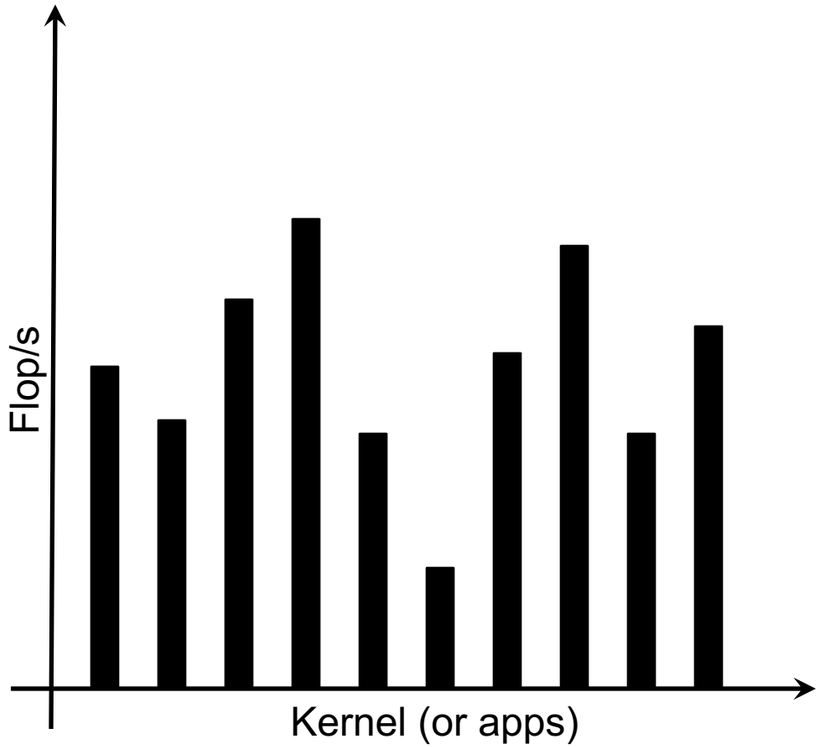
    but 5x the flop rate

```
#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



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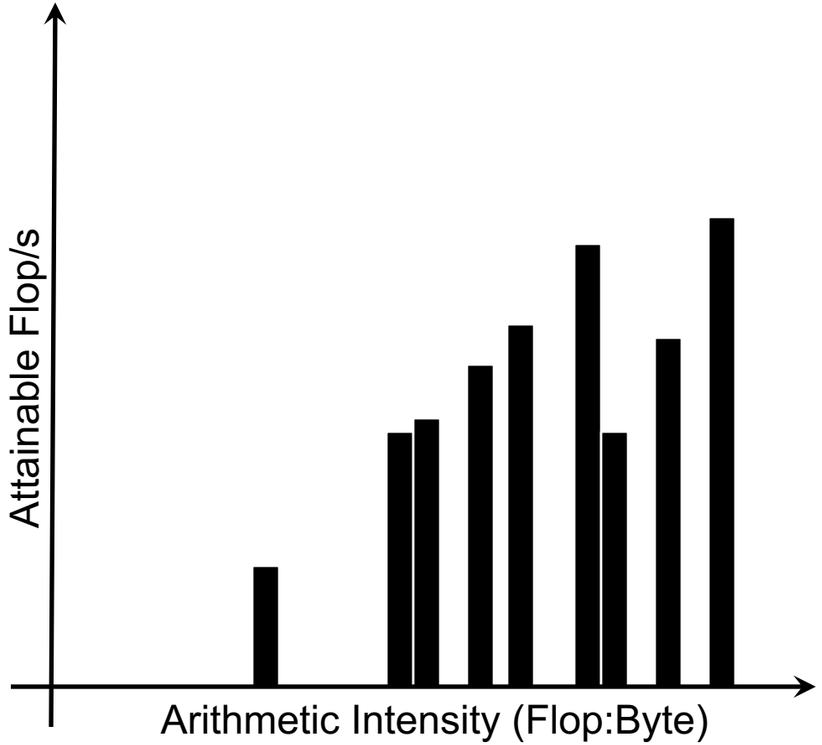
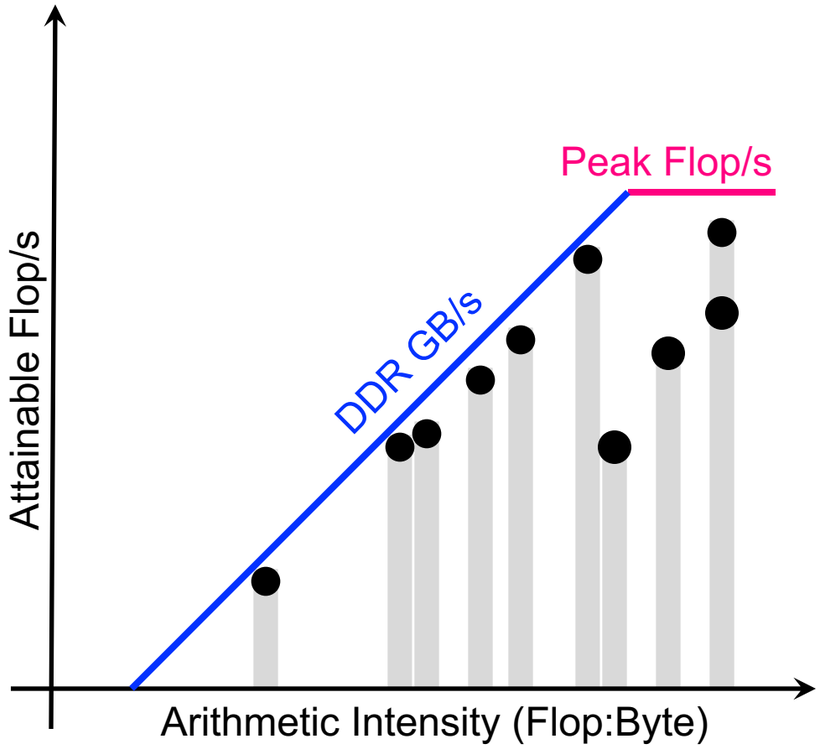
- We can sort kernels by AI …



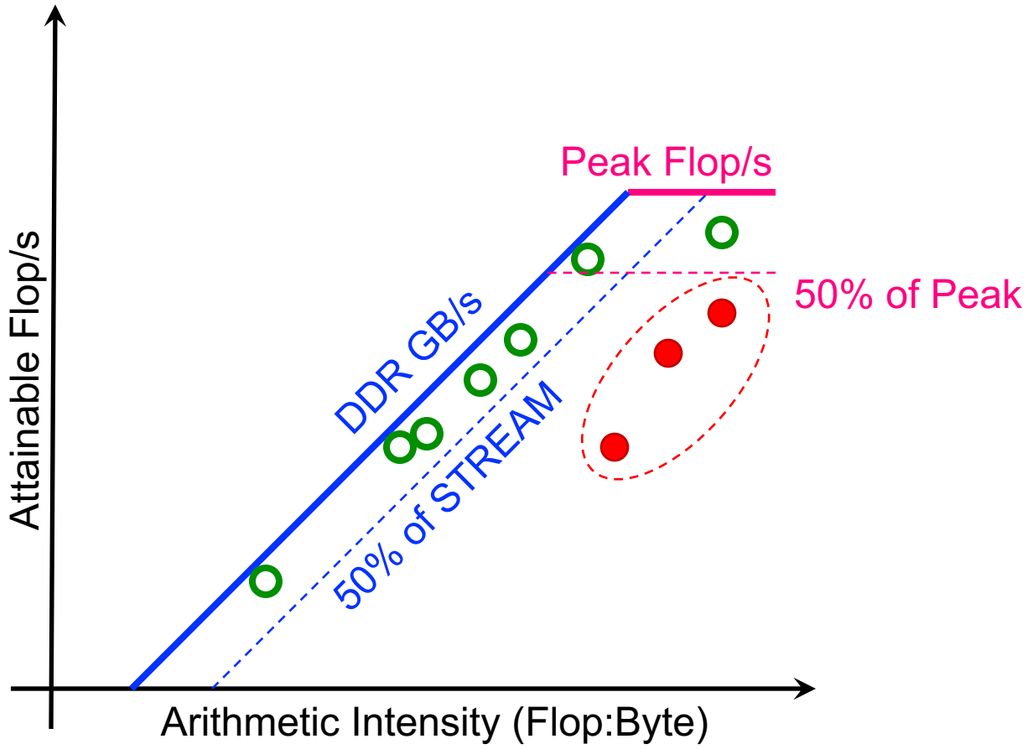
Why is Roofline Useful?

- 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



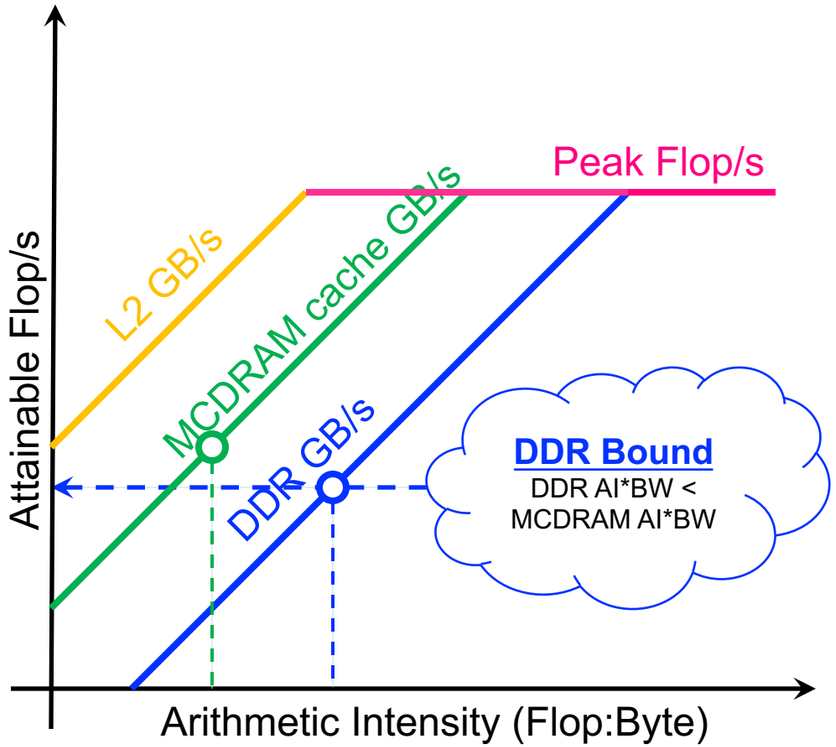
Refining Roofline:
Memory Hierarchy & DLP

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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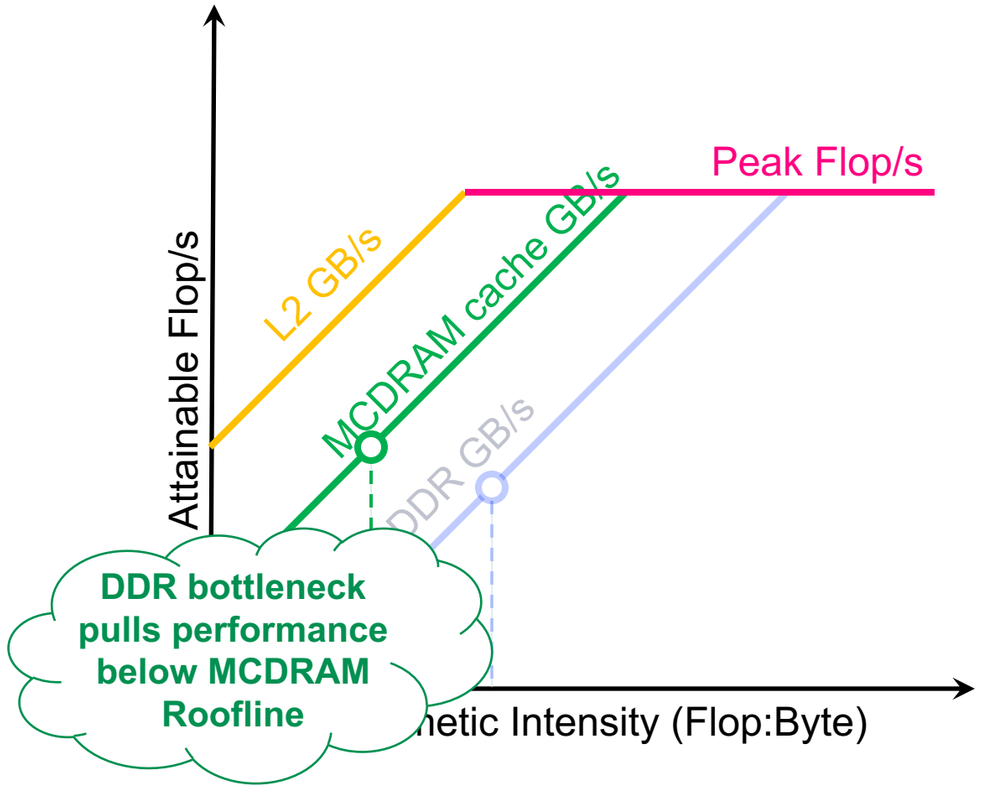

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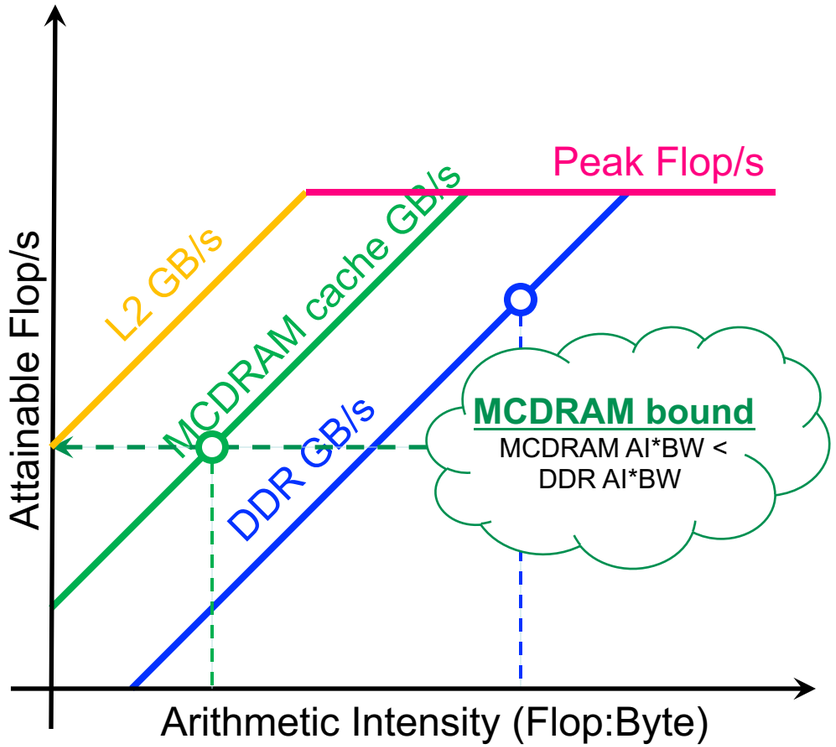

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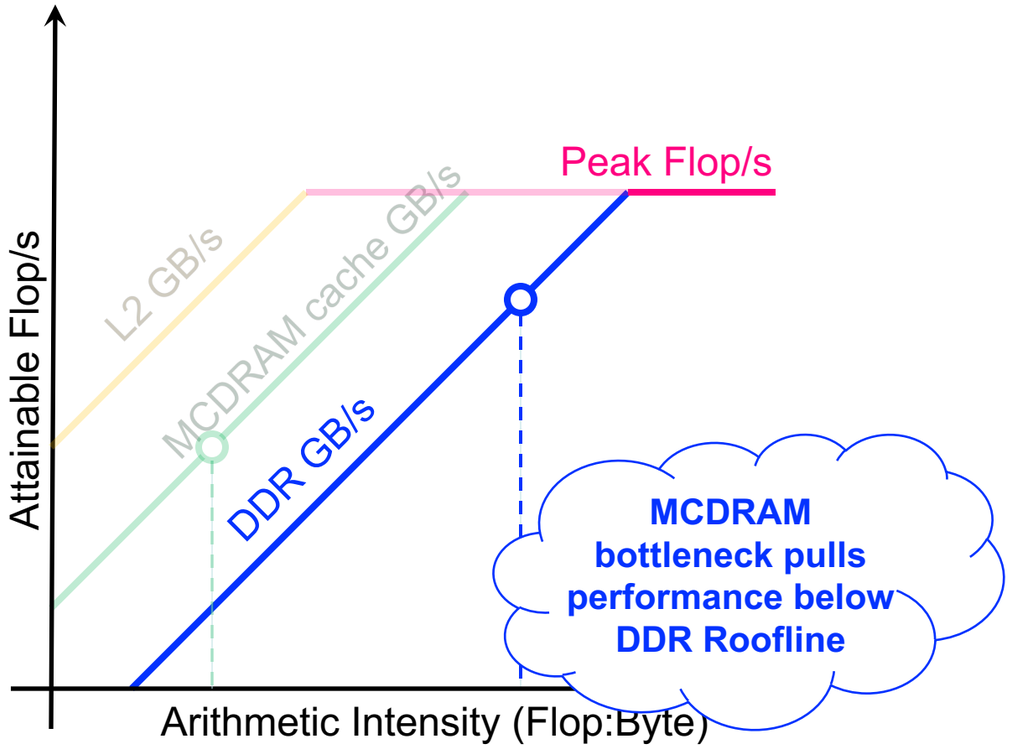
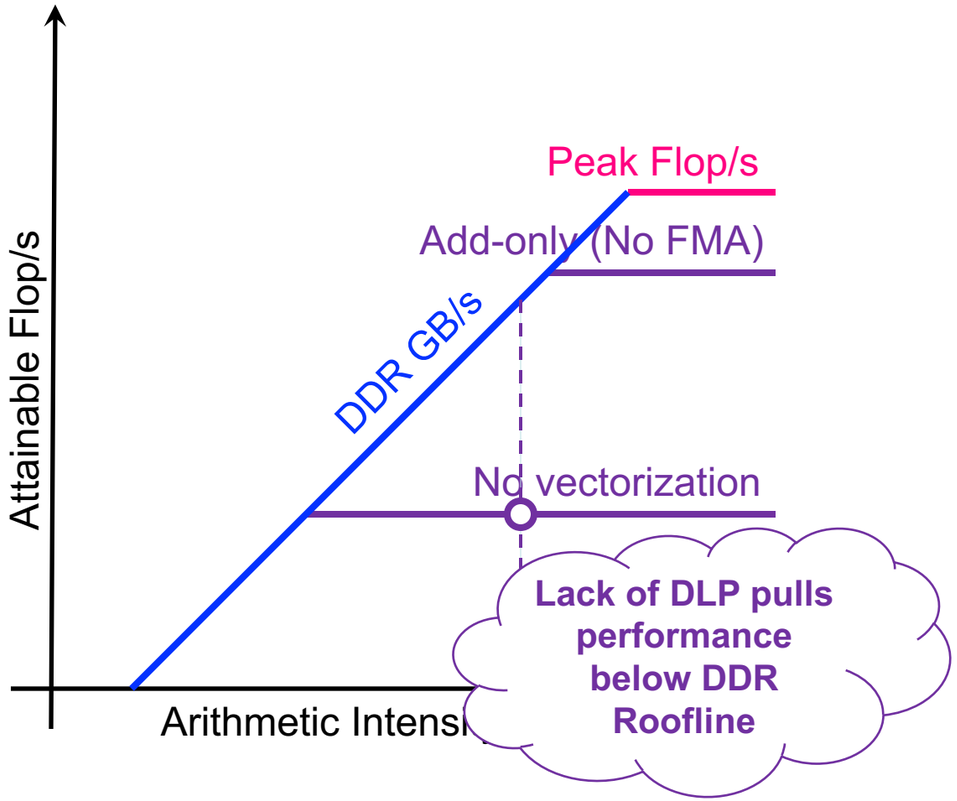


Data, Instruction, Thread-Level Parallelism…

- 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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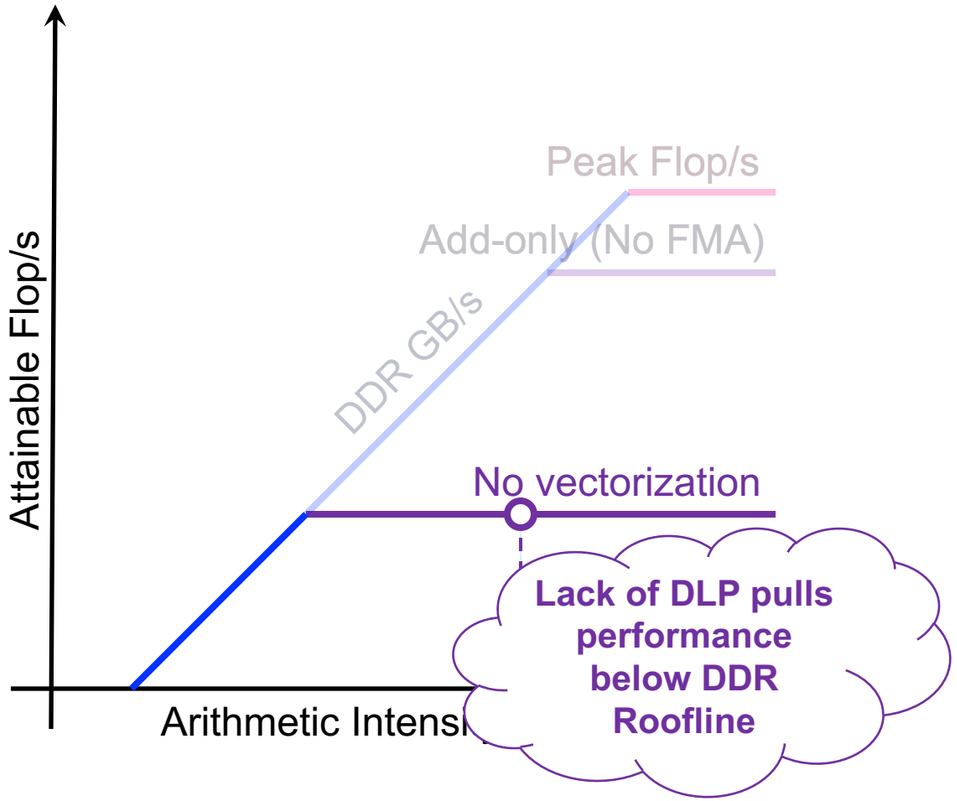
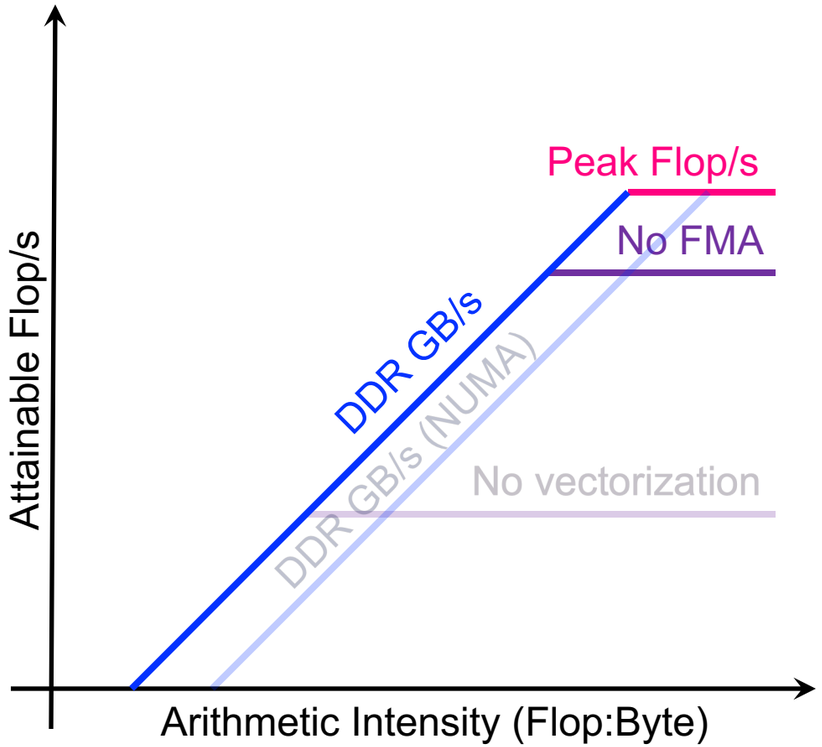


Roofline Model:

Roofline-driven Performance Optimization

Roofline-Driven Performance Optimization

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



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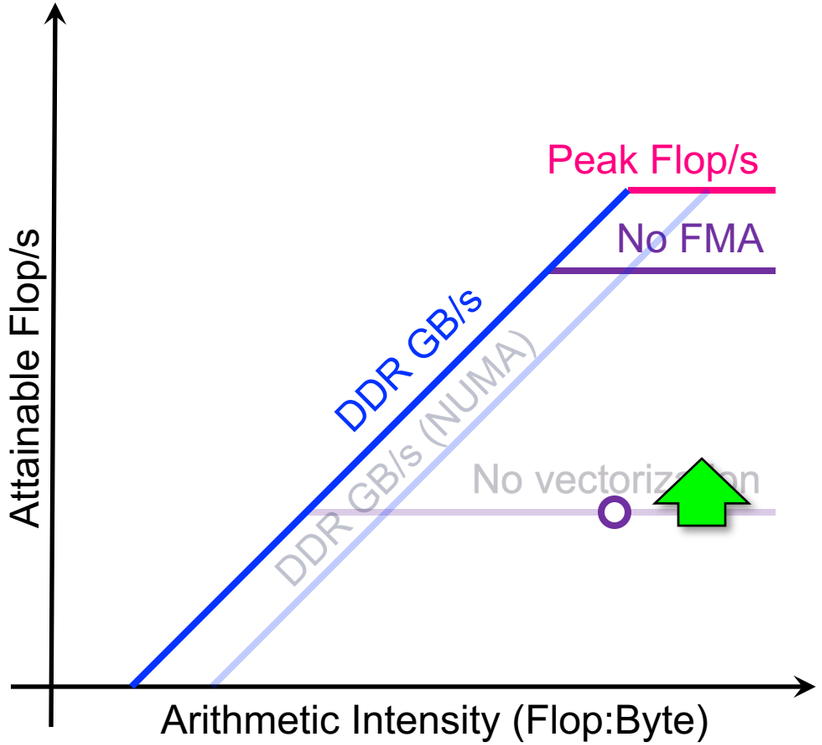

Roofline-Driven Performance Optimization

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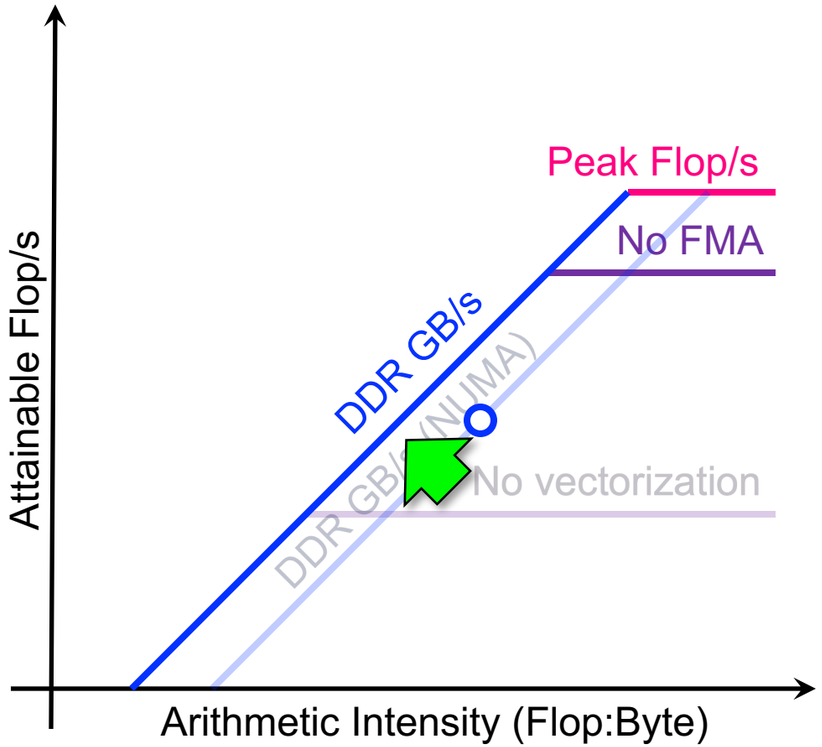

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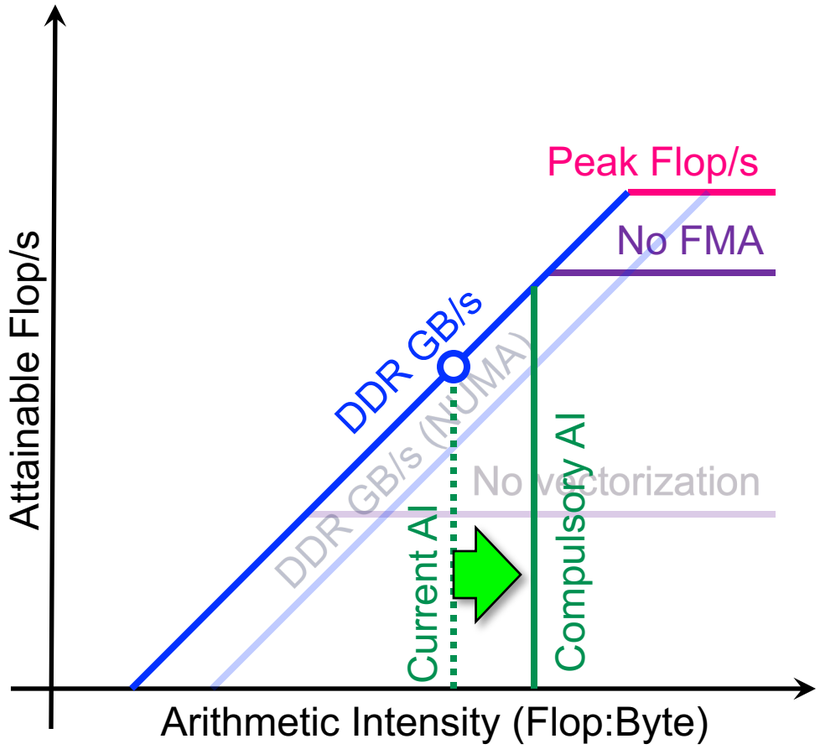
- **Minimize data movement (e.g. cache blocking)**



Roofline In Practice:

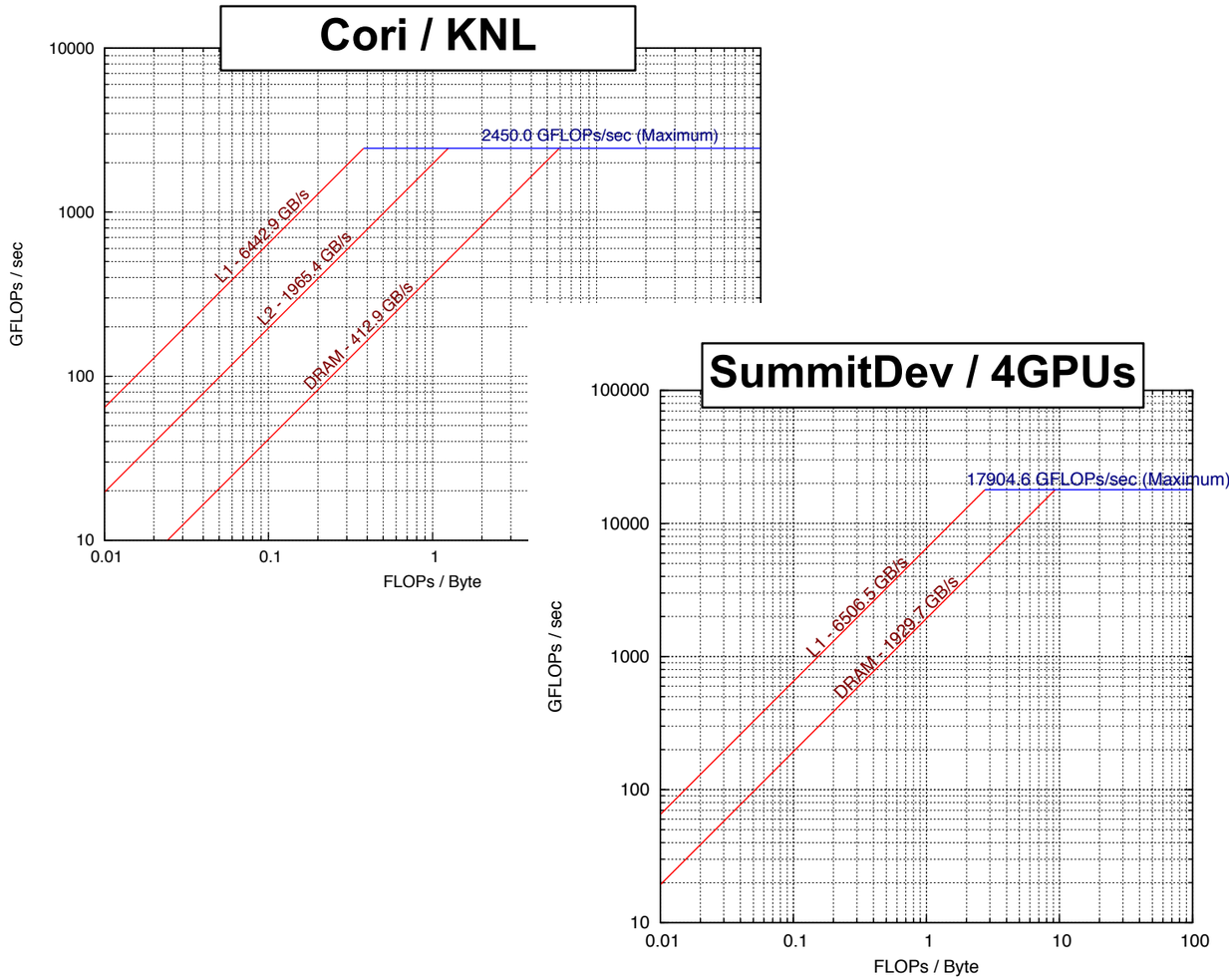
Evolution at LBL / NERSC

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**



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

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Step 2:
Application Characterization

Measuring AI

- To characterize execution with Roofline we need…
  - **Time**
  - **Flops** (=> flop's / time)
  - **Data movement** between each level of memory (=> 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, spare, …)

✗ 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

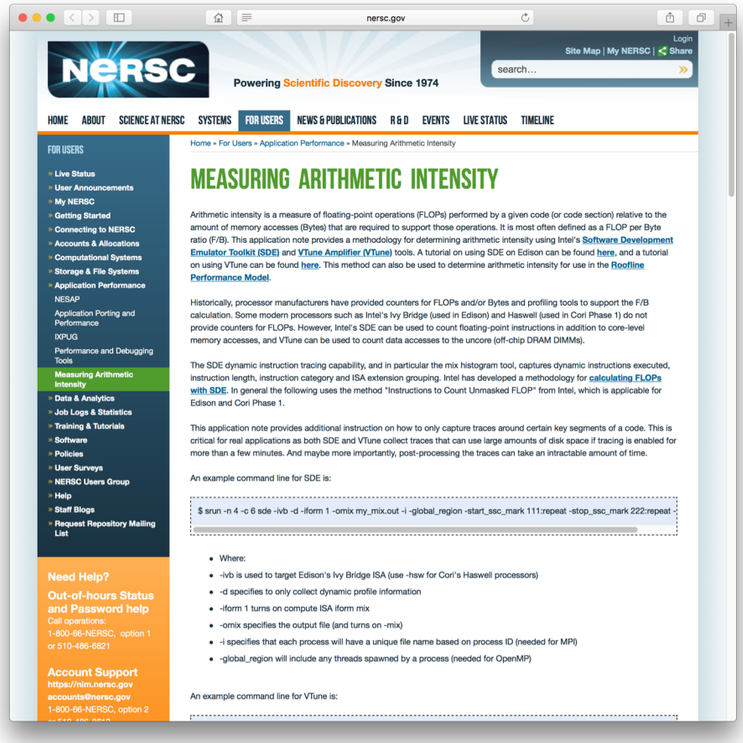
✗ >10x overhead (short runs / reduced concurrency)

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…



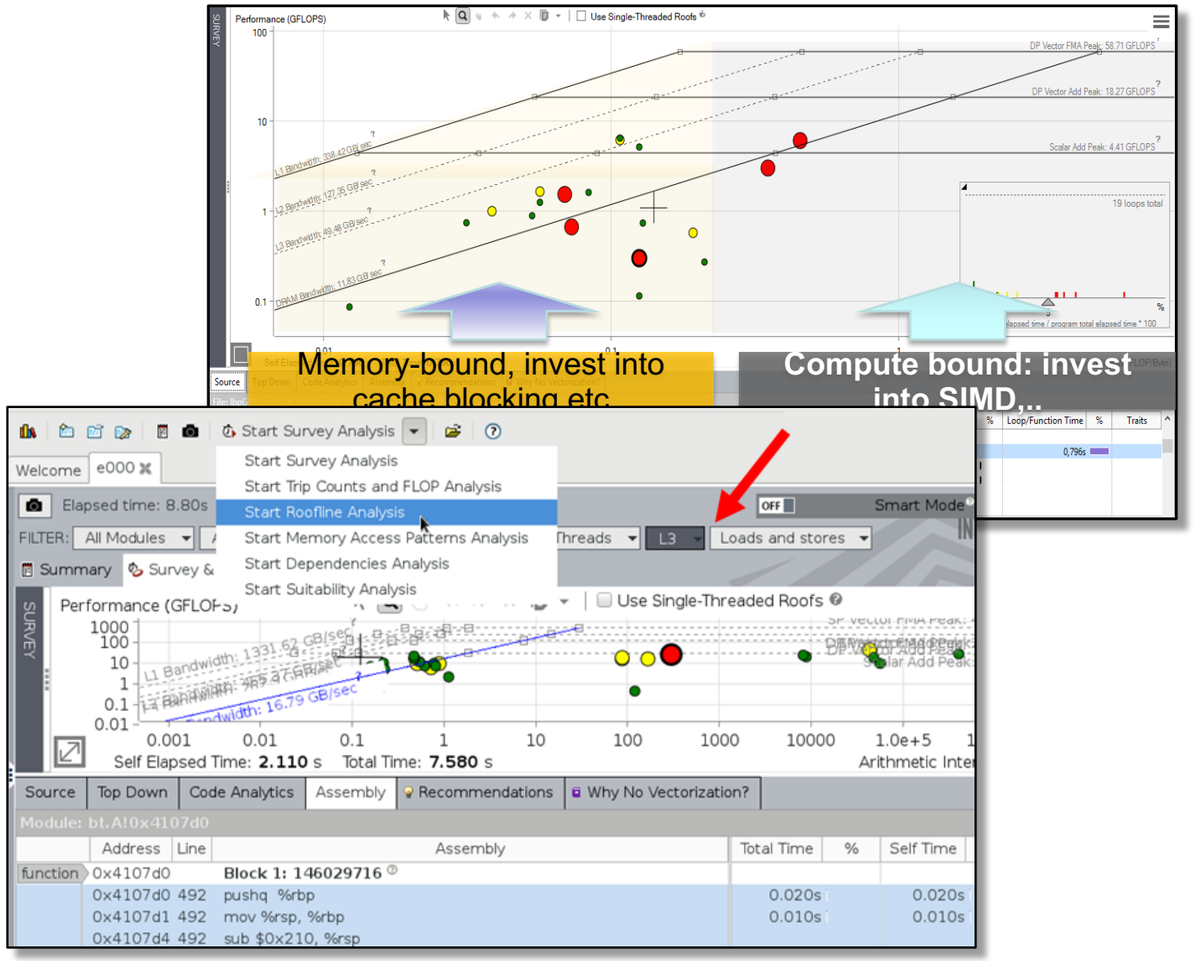
http://www.nersc.gov/users/application-performance/measuring-arithmetic-intensity/

NERSC is LBL's production computing division
CRD is LBL's Computational Research Division
NESAP is NERSC's KNL application readiness project
LBL is part of SUPER (DOE SciDAC3 Computer Science Institute)

BERKELEY LAB

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 Simulator[1] (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

[1]Experimental 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
  - **Ilic 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 looses 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 Roofline[1] (cache simulator) has also been integrated into Intel Advisor

[1]Experimental 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

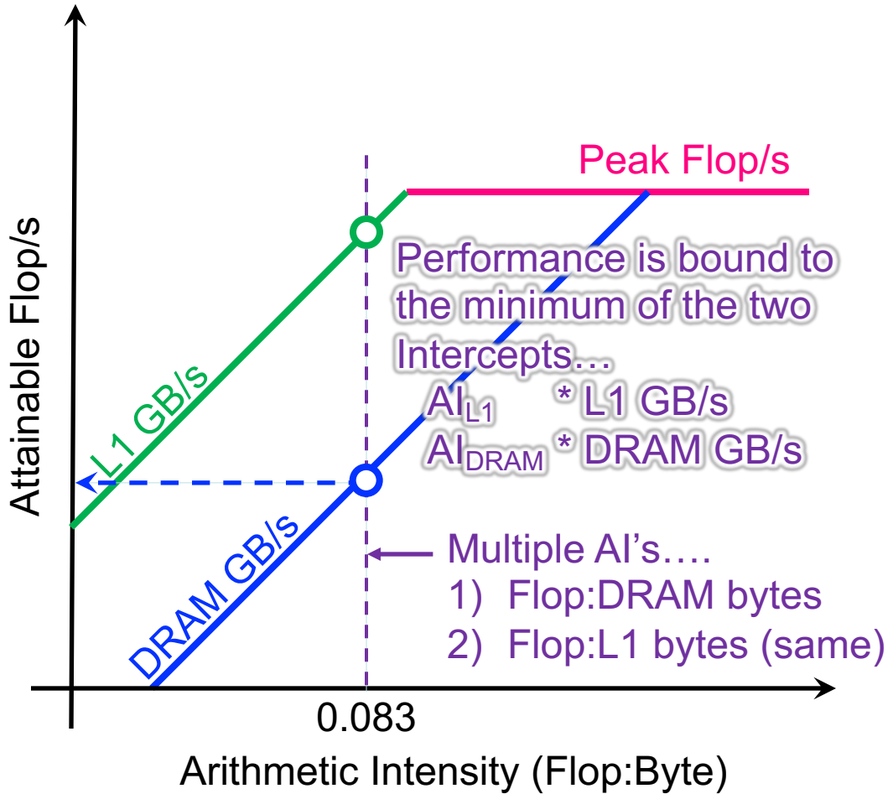
Example: STREAM

- 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+delta for any delta.
- … leads to a DRAM AI equal to the L1 AI

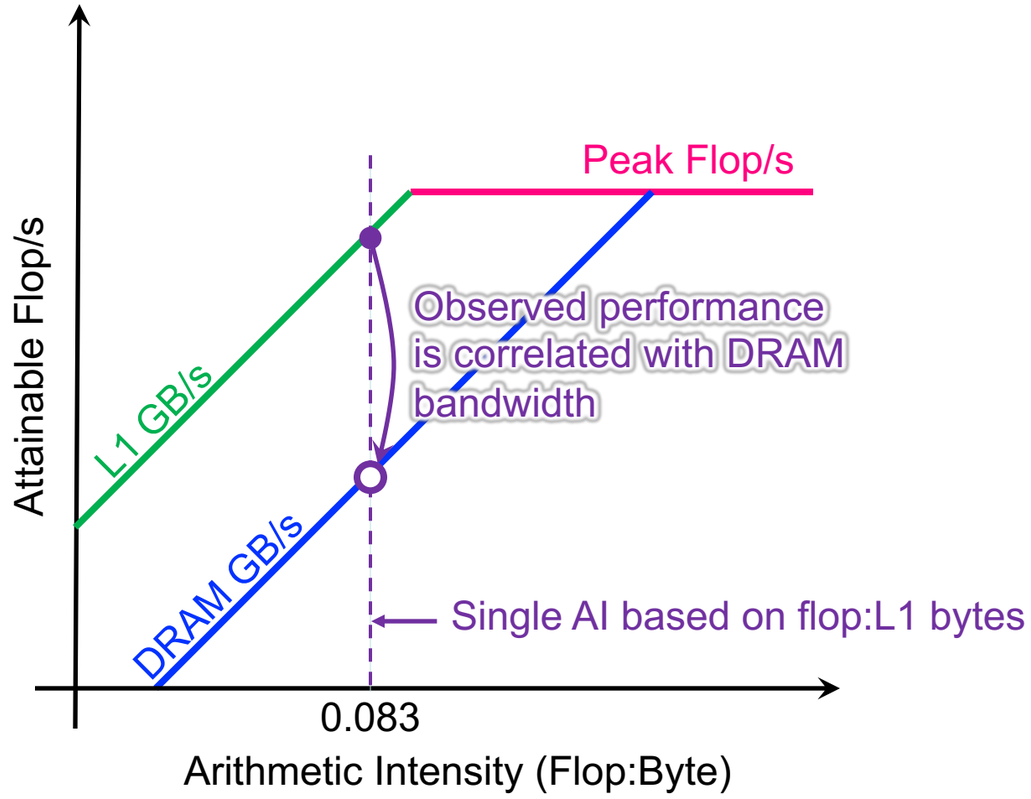
```
#pragma omp parallel for
for(i=0;i<N;i++){
  Z[i] = X[i] + alpha*Y[i];
}
```

Example: STREAM

Hierarchical Roofline



Cache-Aware Roofline



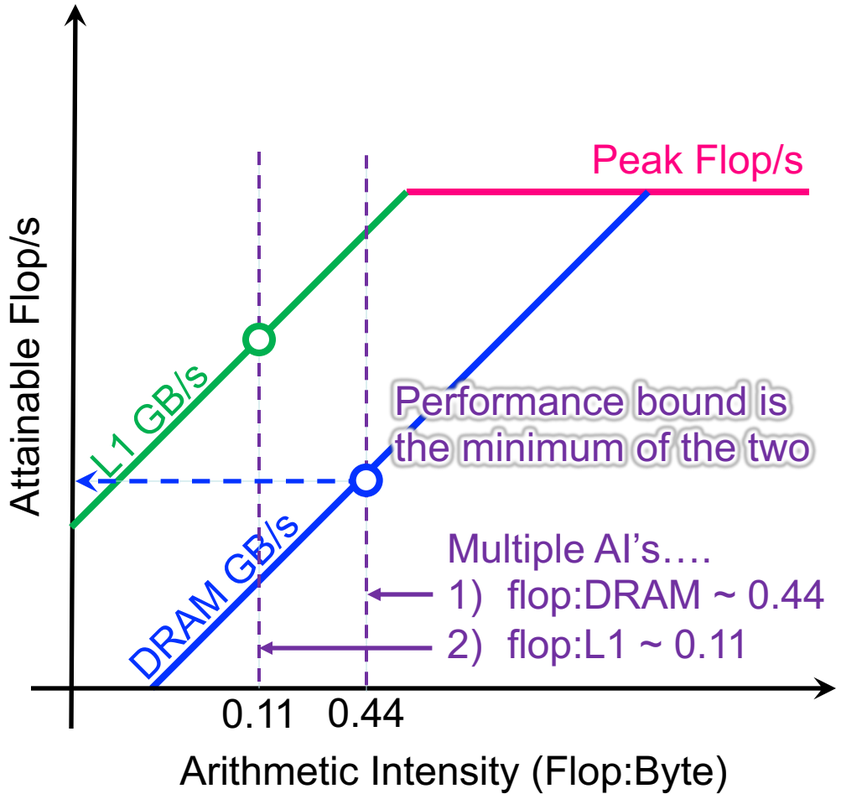
Example: 7-point Stencil (Small Problem)

- 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

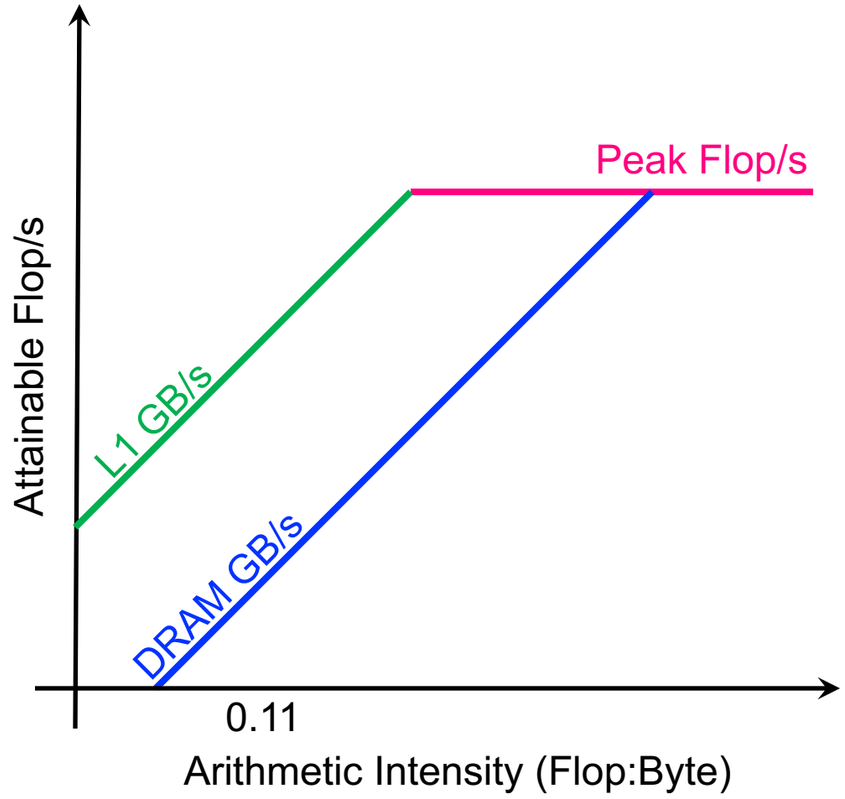
```
#pragma omp parallel for
for(k=1;k<dim+1;k++){
for(j=1;j<dim+1;j++){
for(i=1;i<dim+1;i++){
  new[k][j][i] = -6.0*old[k  ][j  ][i  ]
                     + old[k  ][j  ][i-1]
                     + old[k  ][j  ][i+1]
                     + old[k  ][j-1][i  ]
                     + old[k  ][j+1][i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

Example: 7-point Stencil (Small Problem)

Hierarchical Roofline



Cache-Aware Roofline



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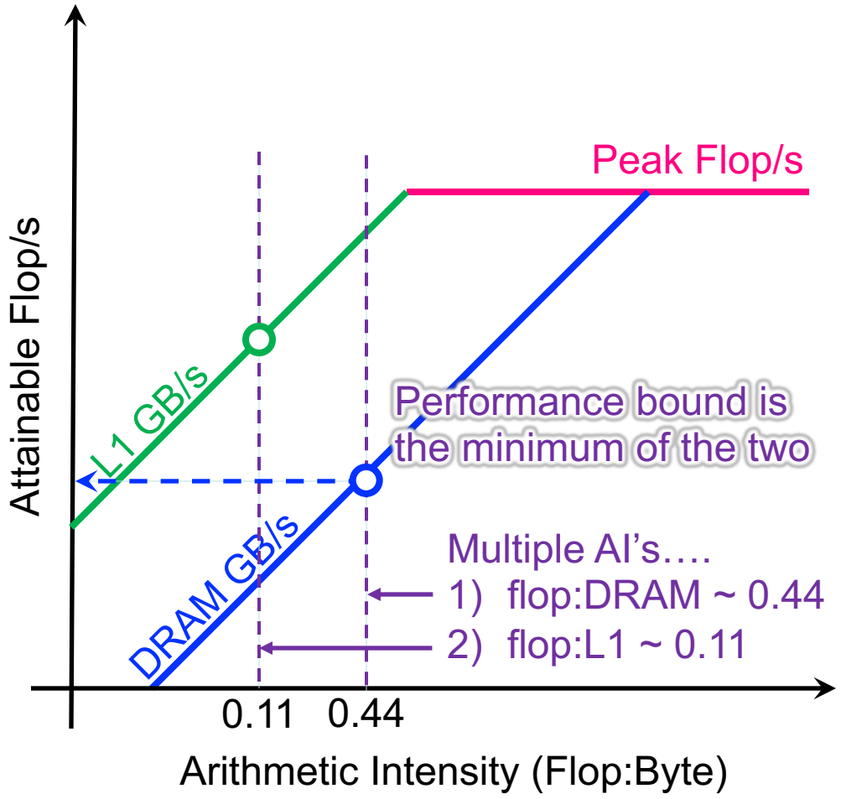
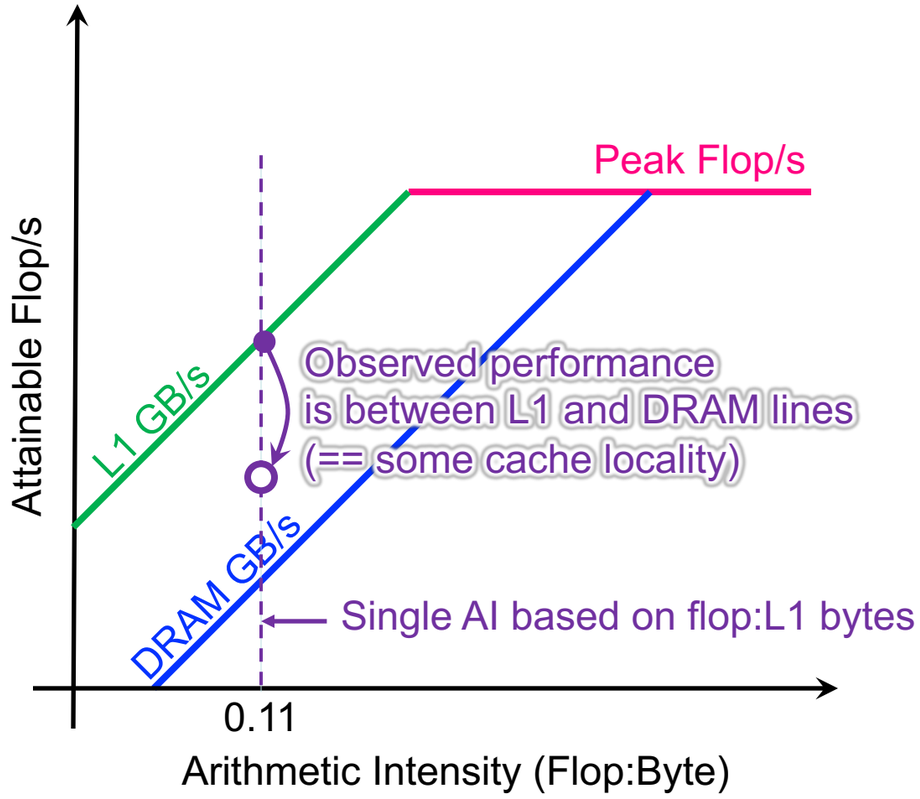
Hierarchical Roofline

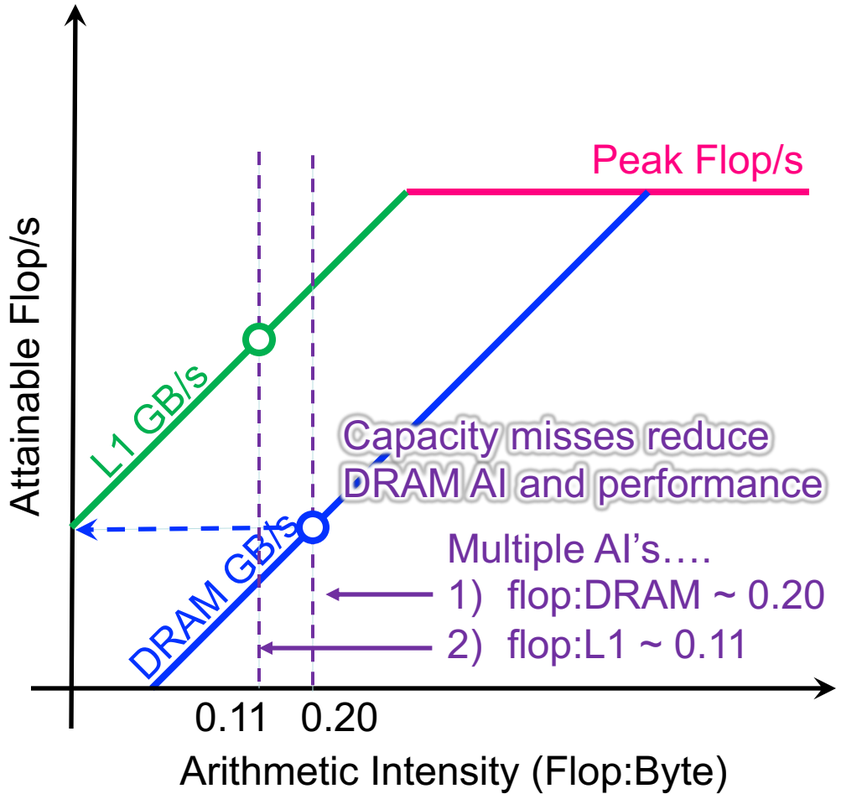


Cache-Aware Roofline



Example: 7-point Stencil (Large Problem)

Hierarchical Roofline



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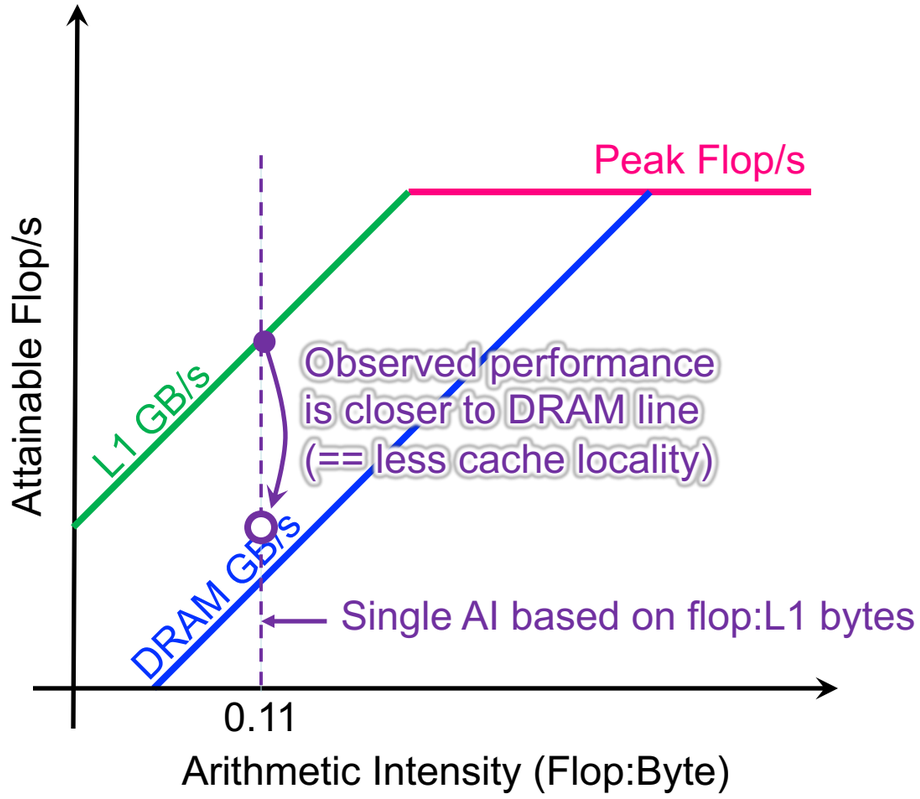
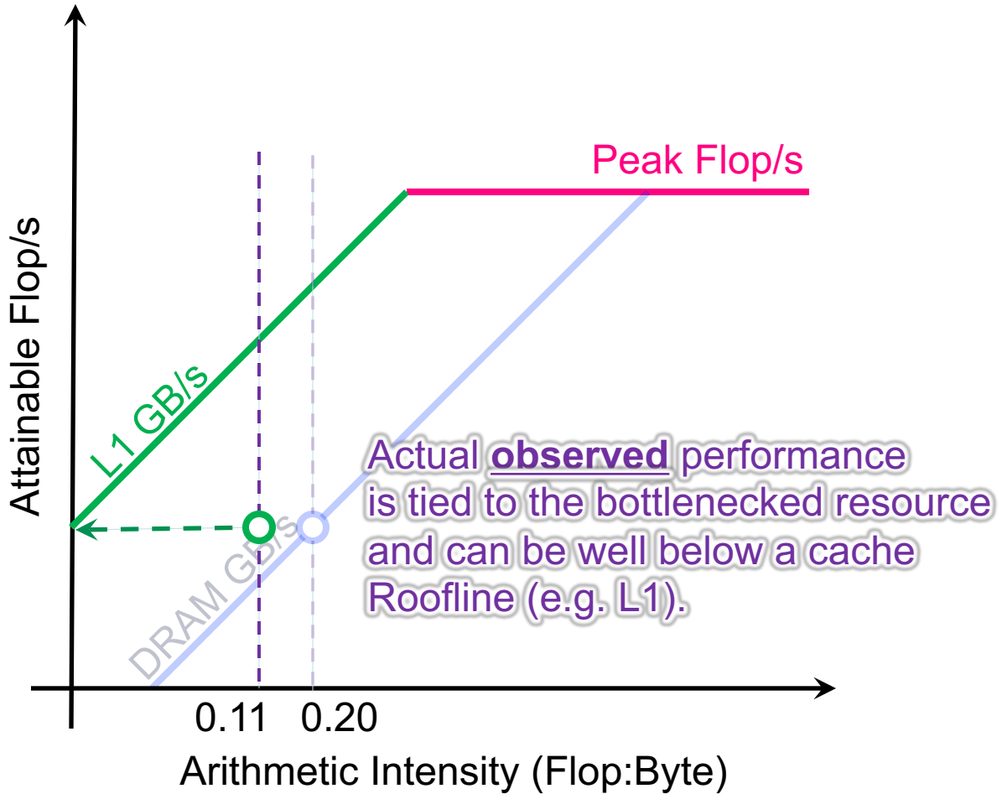


Example: 7-point Stencil (Observed Perf.)

Hierarchical Roofline



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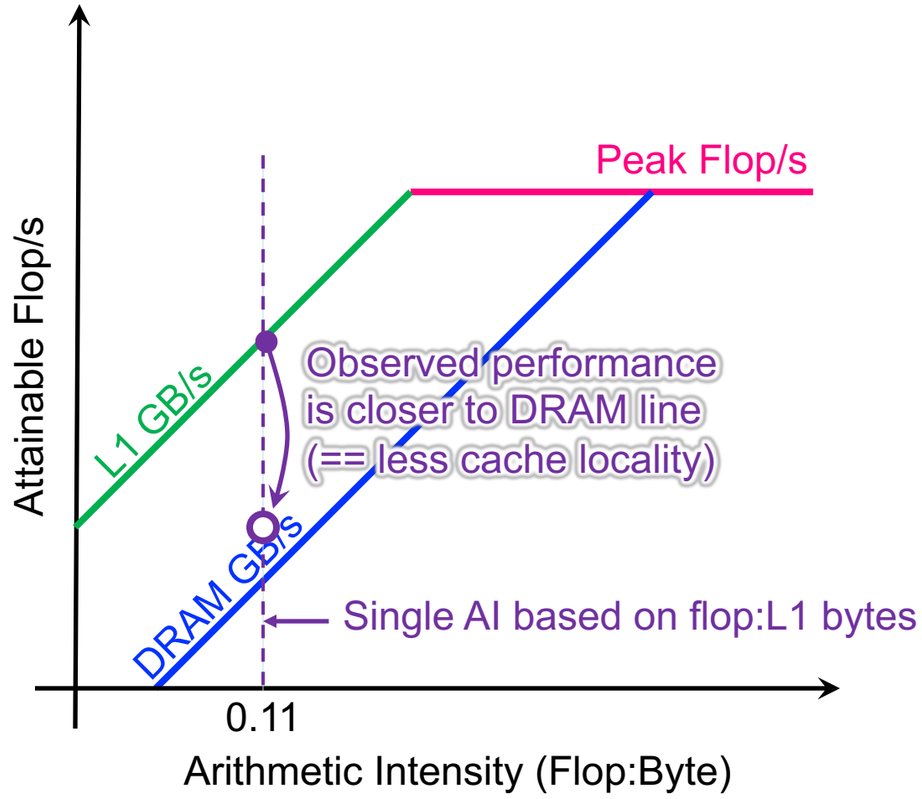

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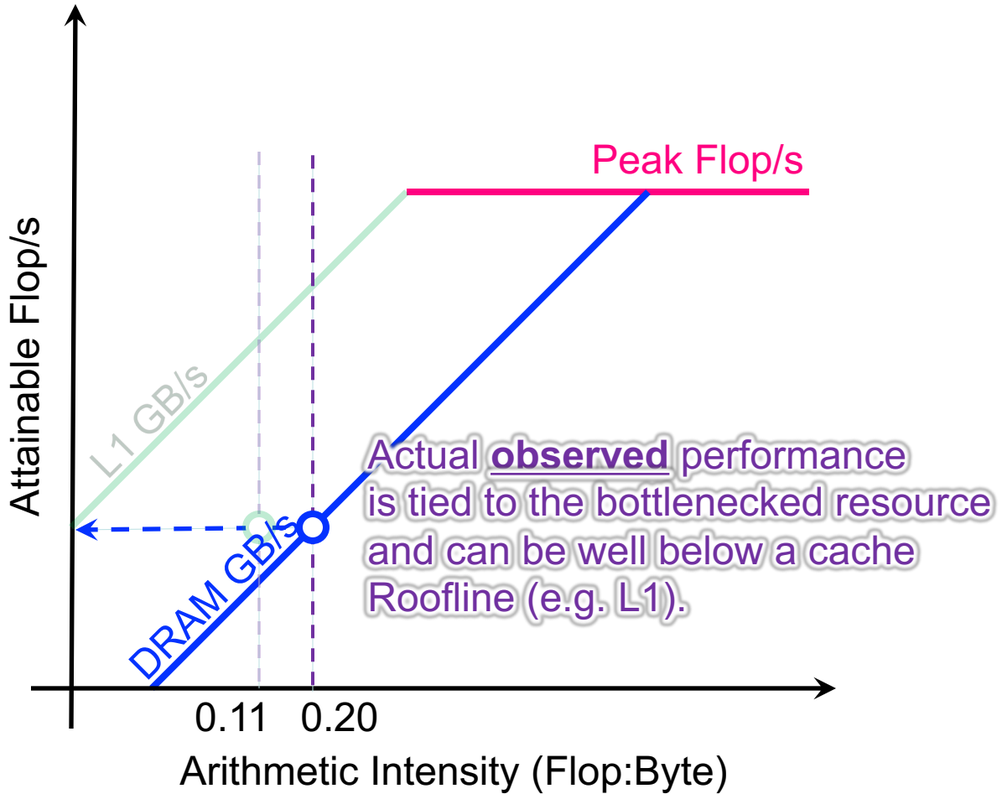
Hierarchical Roofline



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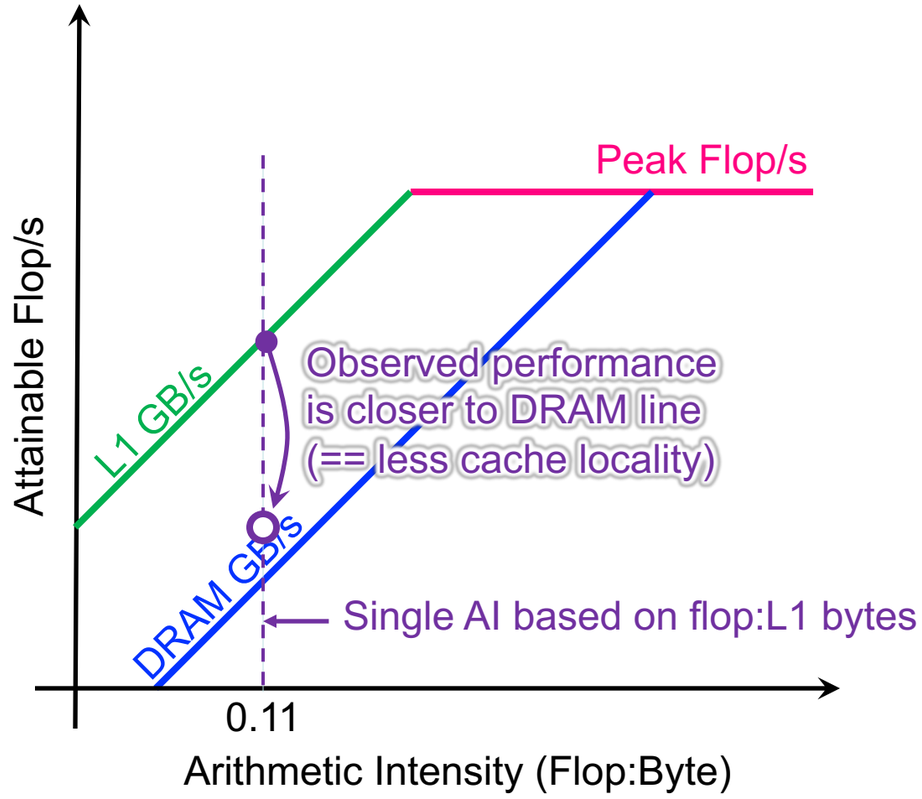


Questions?

Don’t forget to take the Survey…

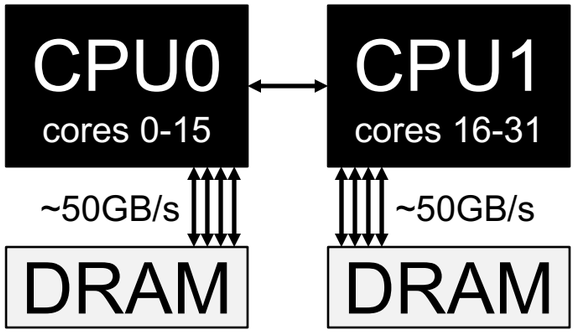
http://bit.ly/sc18-eval

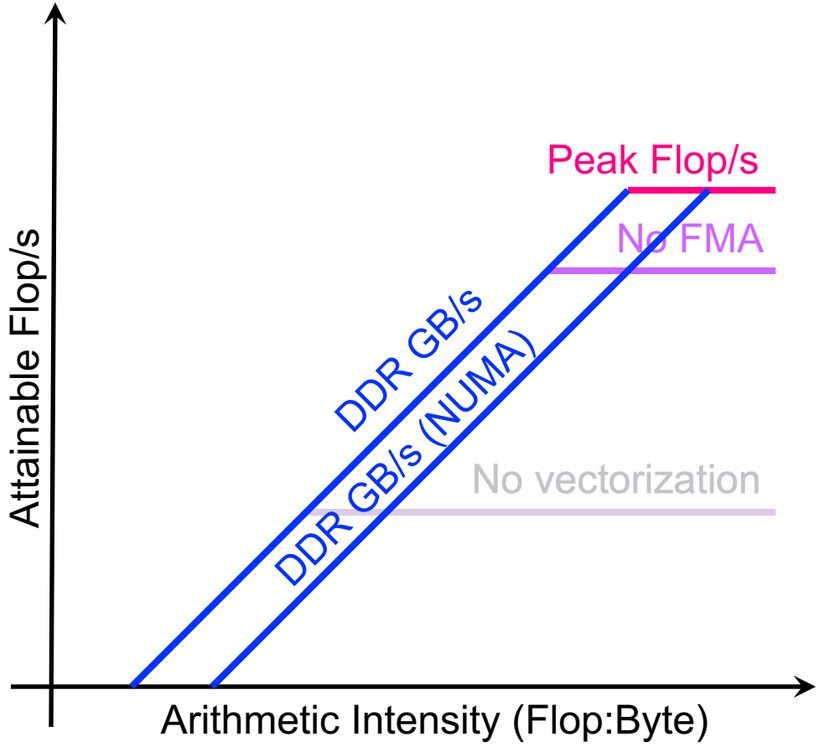
Backup

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

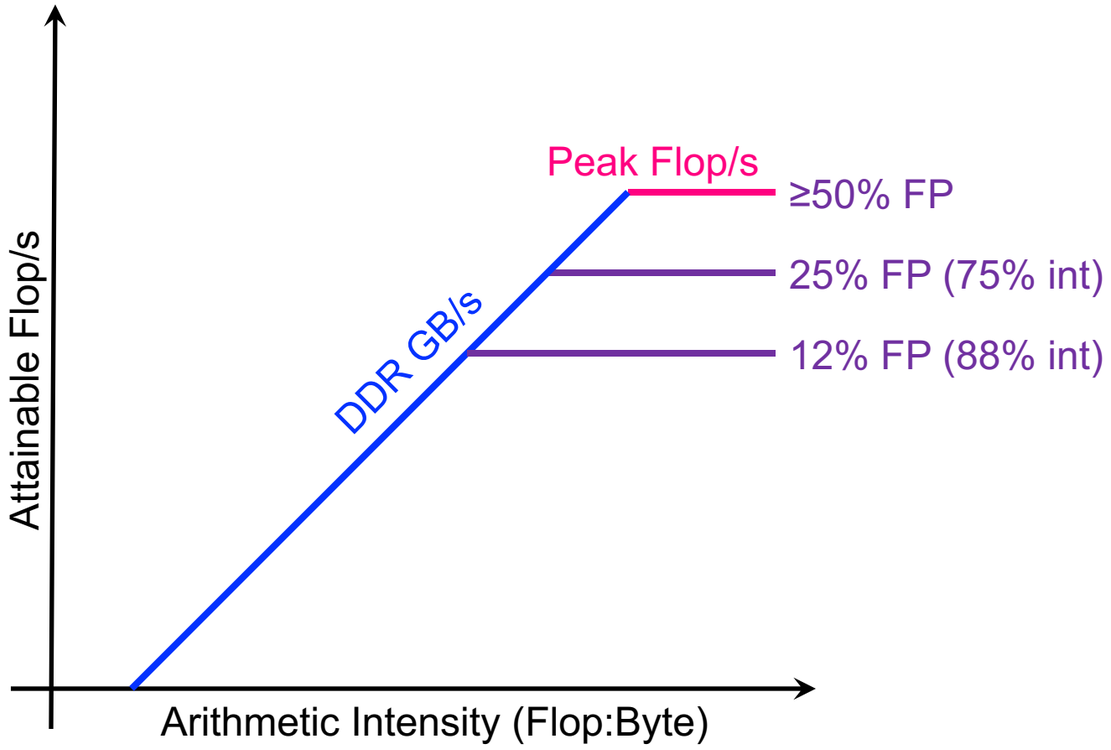




Refining Roofline:
Instruction Issue Bandwidth

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



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- e.g. Haswell
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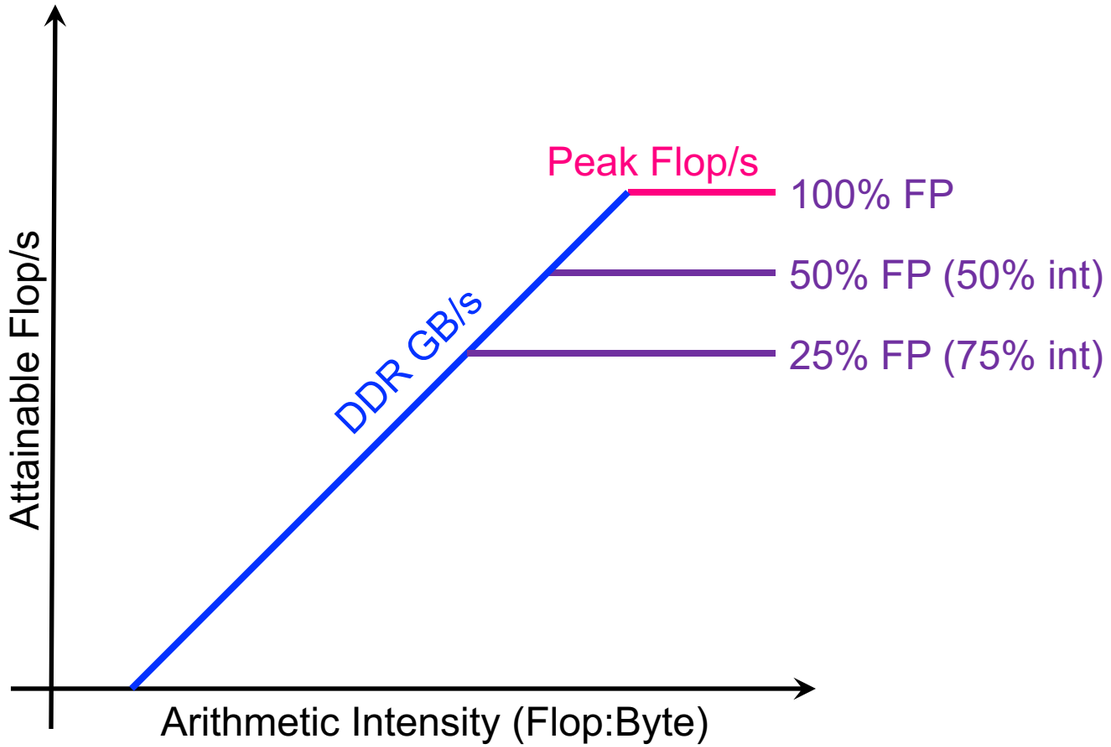
- e.g. KNL
  - 2-issue superscalar
  - 2 FP data paths
  - Requires 100% of the instructions to be FP to get peak performance



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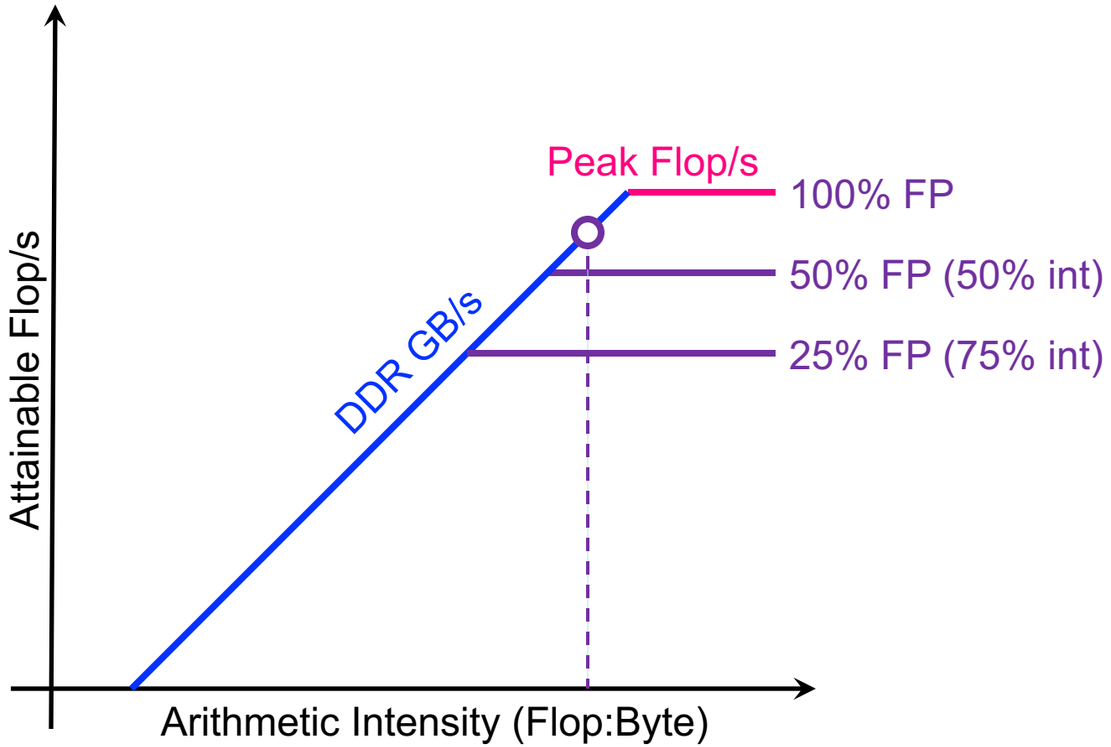

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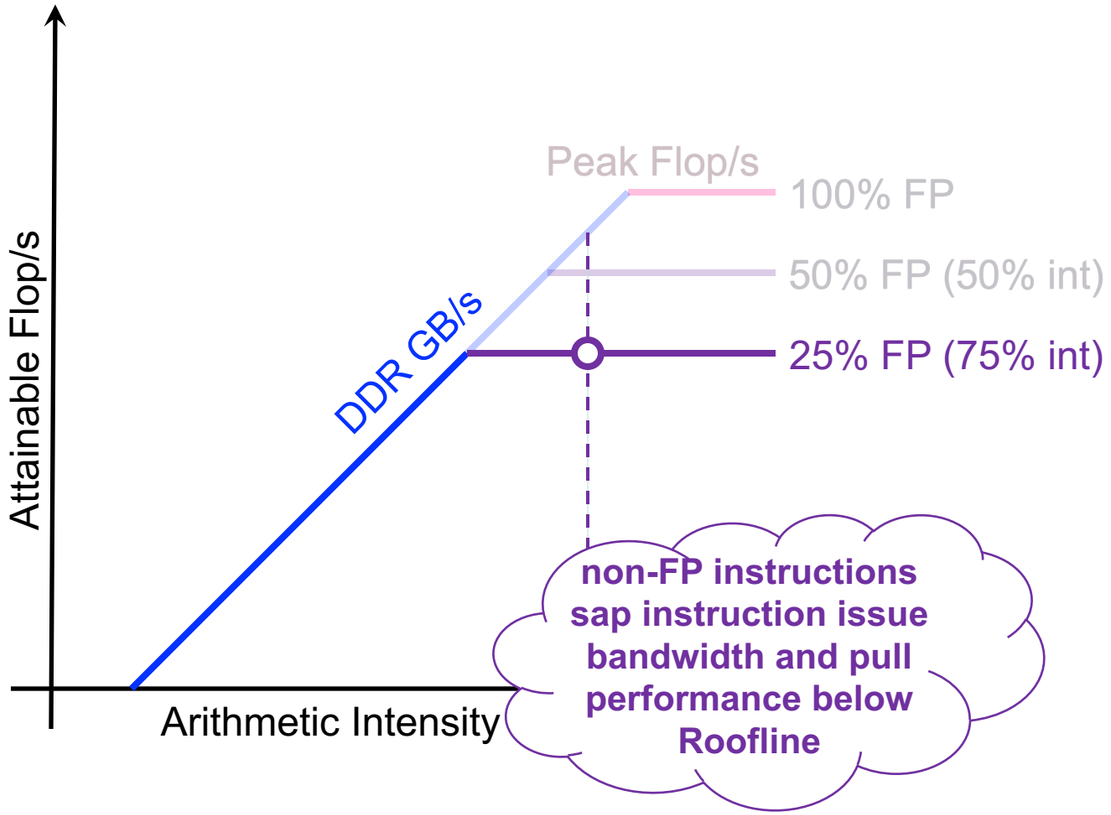
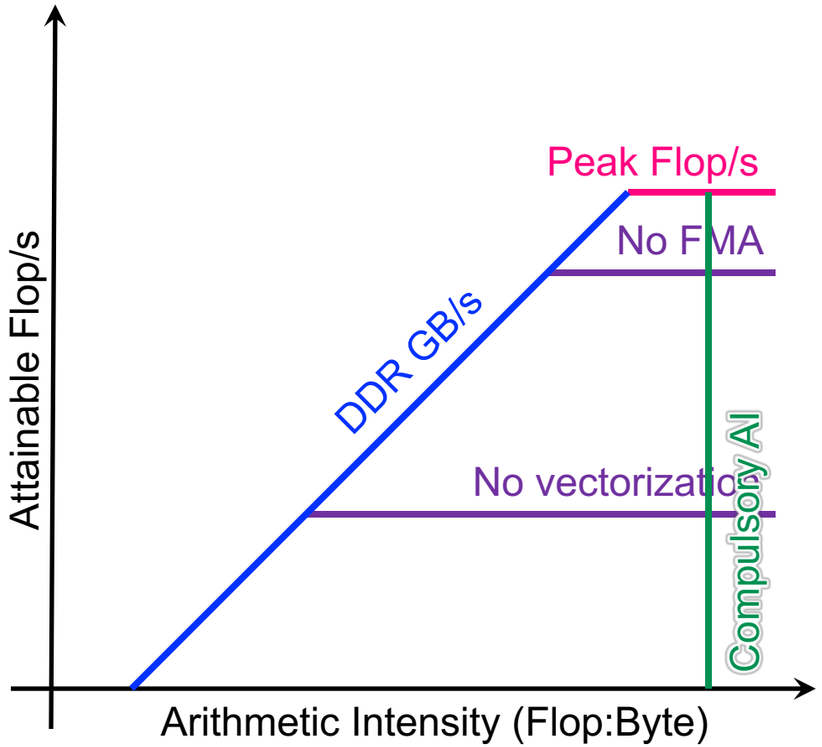


Refining Roofline:

Compulsory, Capacity, and Conflict misses

Locality Walls

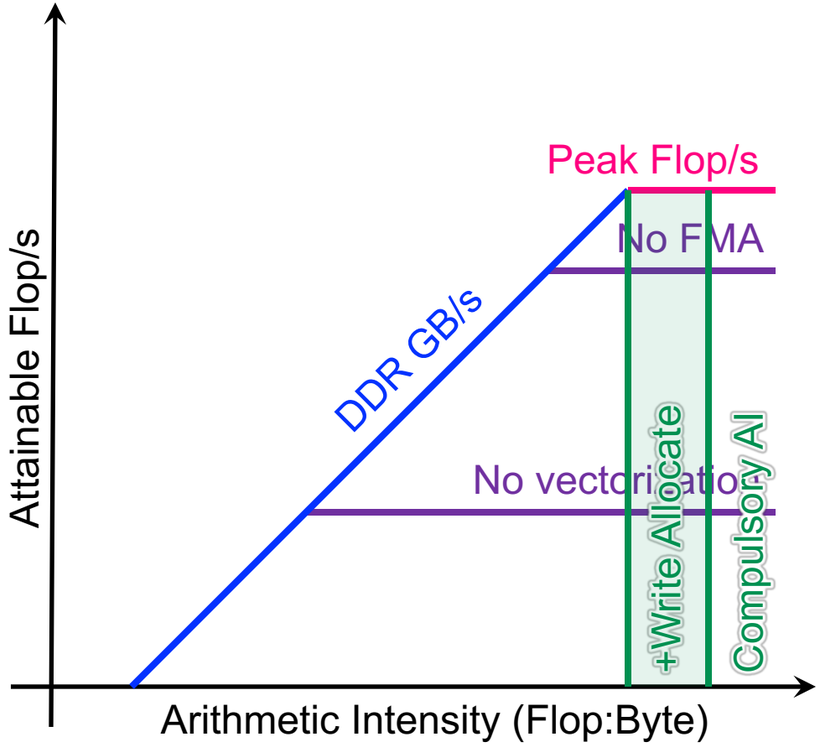
- Naively, we can bound AI using only compulsory cache misses



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

Locality Walls

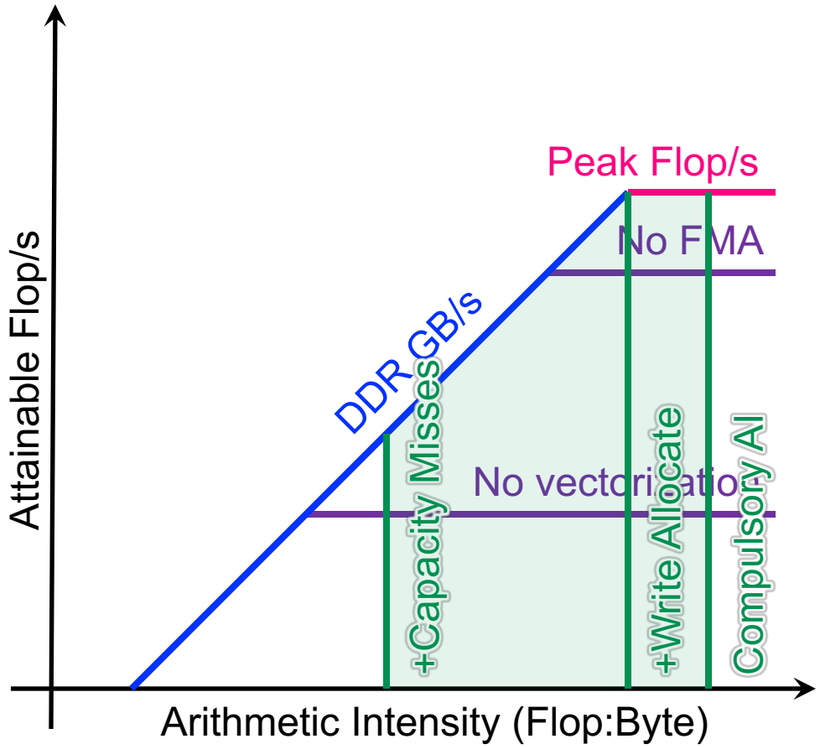
- Naively, we can bound AI using only compulsory cache misses
- However, write allocate caches can lower AI



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

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



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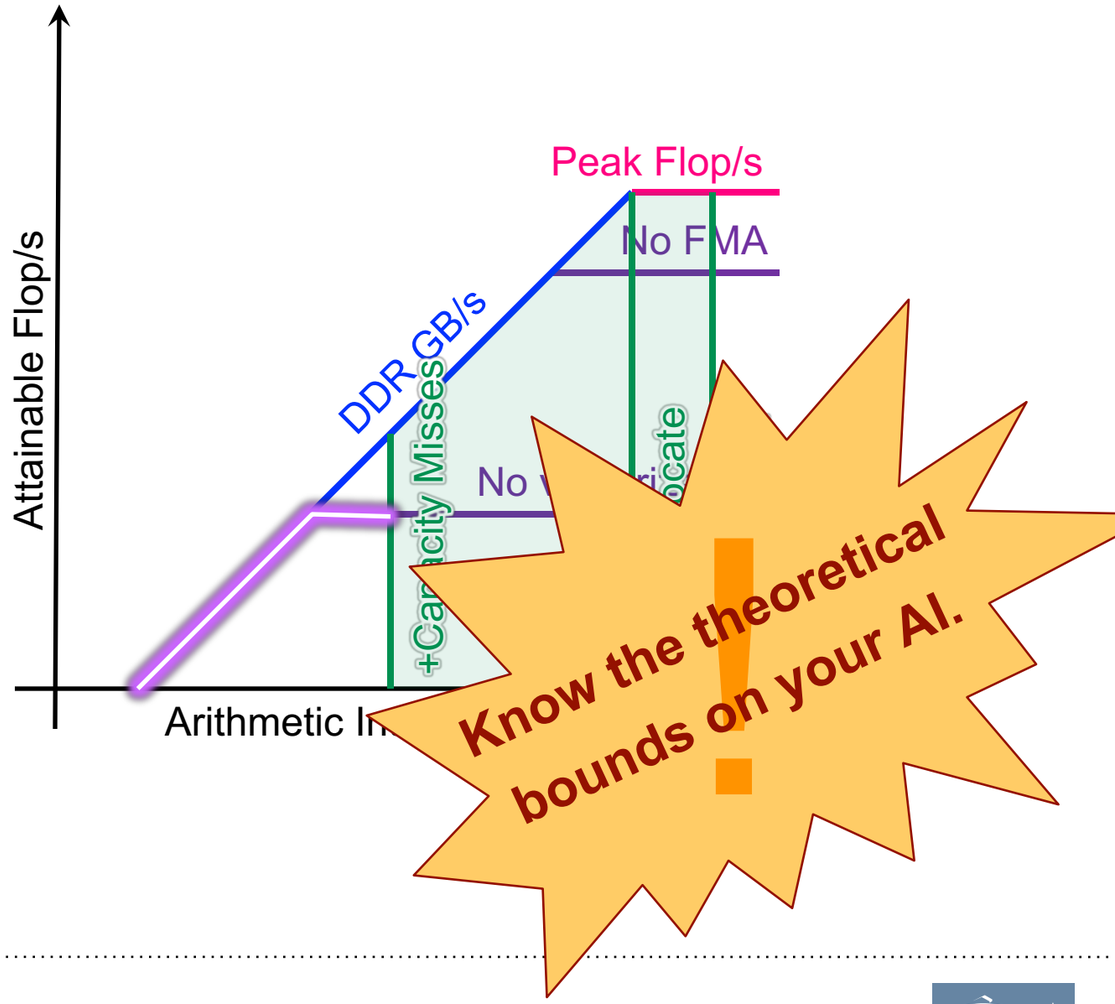
Locality Walls

- 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**

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



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