NORTHWEST INSTITUTE for ADVANCED COMPUTING

# AMATH 483/583
# High Performance Scientific Computing

# Lecture 8:
# BLAS, Strassen’s Algorithm, Roofline Model

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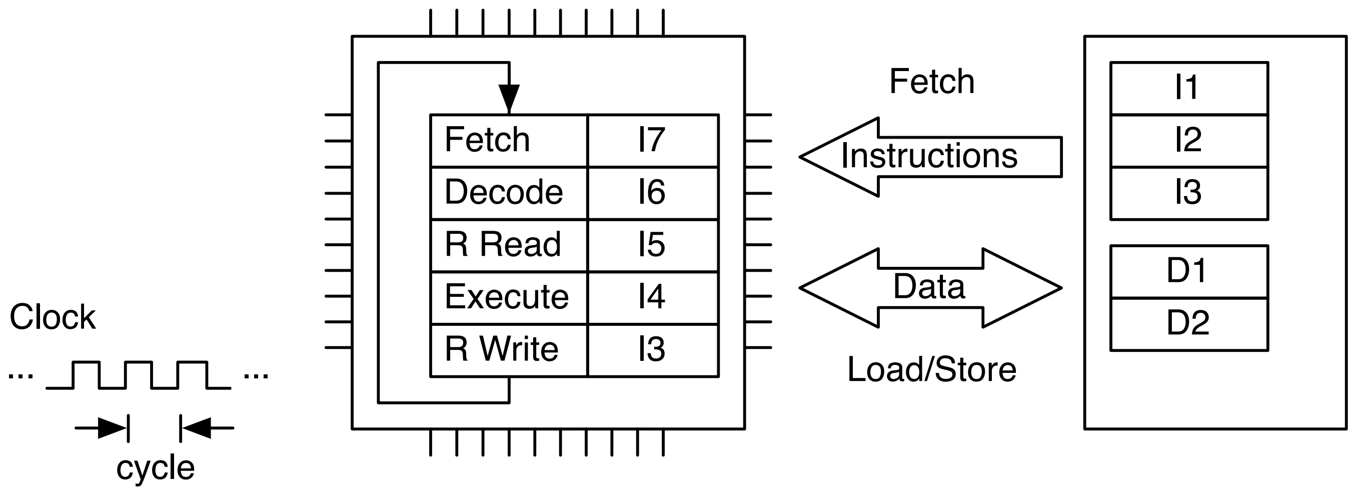
# Overview

- Finish SIMD
- Revisit pipelining, hoisting, copying
- BLAS
- Strassen's Algorithm
- Roofline Model

# Processor Core Instruction Handling

- By pipelining, multiple instructions can be executed at each clock cycle
- Form of instruction-level parallelism (ILP)



# Performance-Oriented Architecture Features

- Execution Pipeline
  - Stages of functionality to process issued instructions
  - Hazards are conflicts with continued execution
  - Forwarding supports closely associated operations exhibiting precedence constraints
- Out of Order Execution
  - Uses reservation stations
  - Hides some core latencies and provide fine grain asynchronous operation supporting concurrency
- Branch Prediction
  - Permits computation to proceed at a conditional branch point prior to resolving predicate value
  - Overlaps follow-on computation with predicate resolution
  - Requires roll-back or equivalent to correct false guesses
  - Sometimes follows both paths, and several deep

Unrolling and inlining can help these

But compilers are really good at that

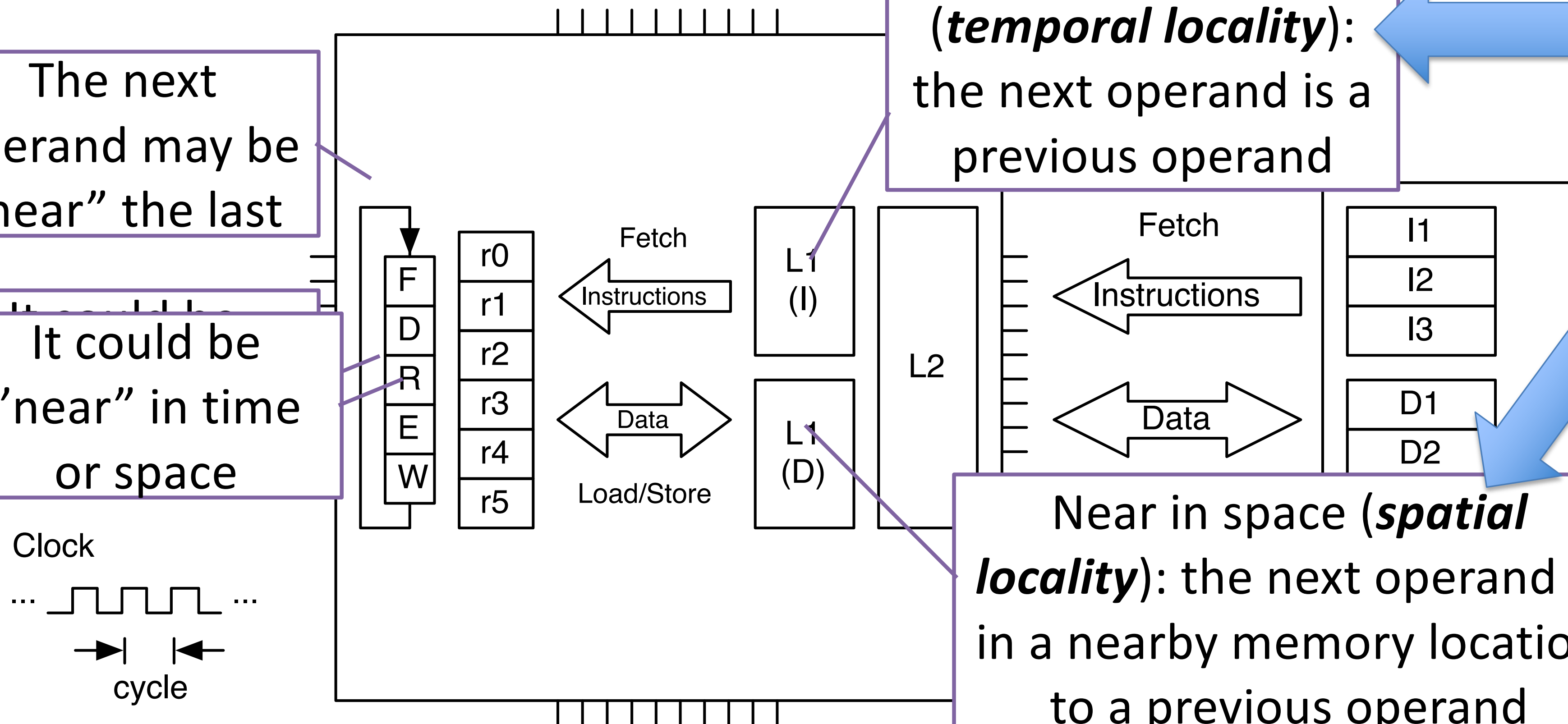
# Locality → Strategy

The next operand may be "near" the last

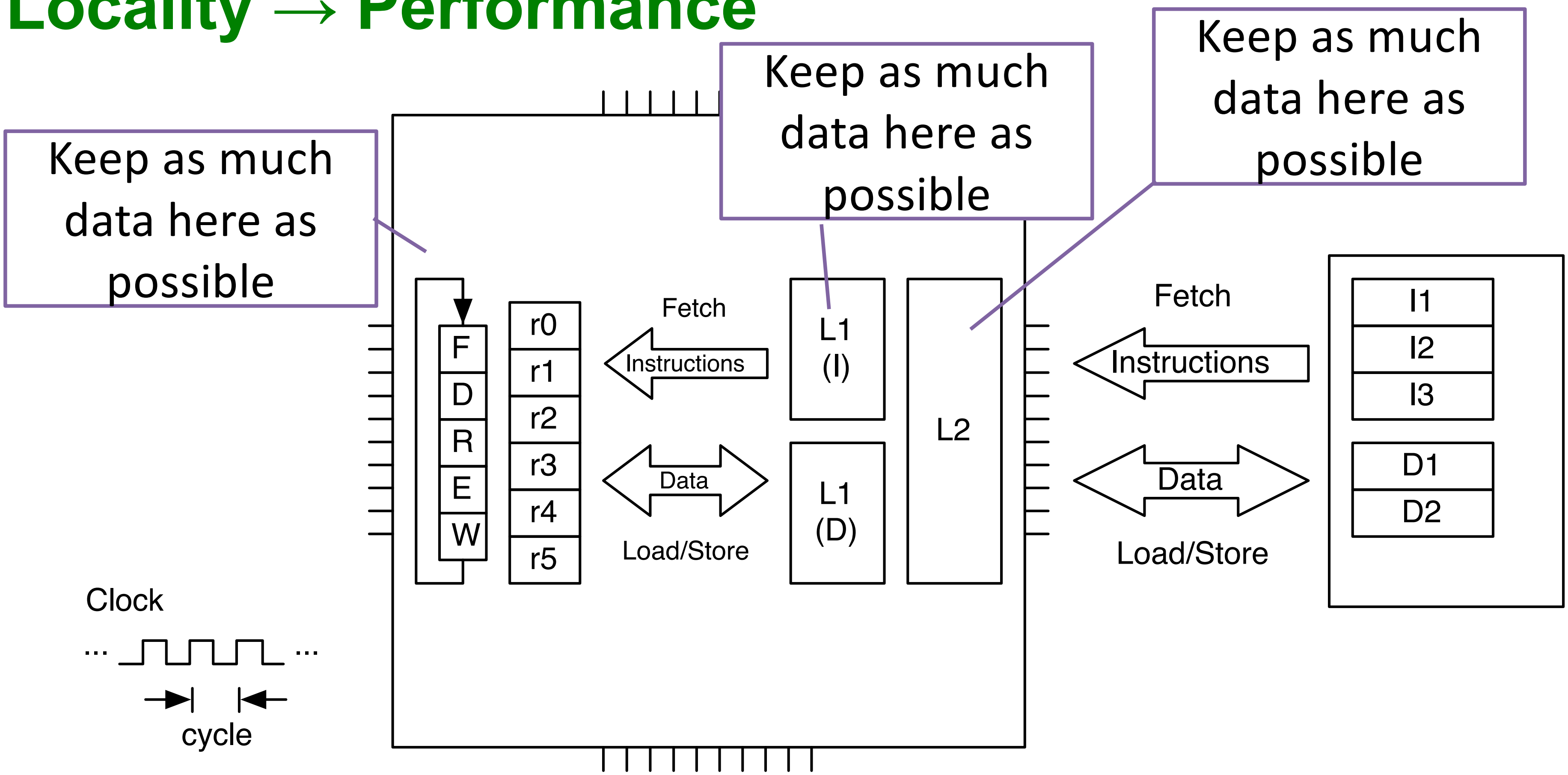
It could be "near" in time or space

Near in time (***temporal locality***): the next operand is a previous operand

Near in space (***spatial locality***): the next operand is in a nearby memory location to a previous operand



# Locality → Performance



# Our Matrix class

Matrix.hpp

```
class Matrix {
public:
  Matrix(size_t M, size_t N) : num_rows_(M), num_cols_(N), storage_(num_rows_ * num_cols_) {}

        double& operator()(size_t i, size_t j)       { return storage_[i * num_cols_ + j]; }
  const double& operator()(size_t i, size_t j) const { return storage_[i * num_cols_ + j]; }

  size_t num_rows() const { return num_rows_; }
  size_t num_cols() const { return num_cols_; }

private:
  size_t              num_rows_, num_cols_;
  std::vector<double> storage_;
};
```

Overloaded operator()

# Just For Benchmarking

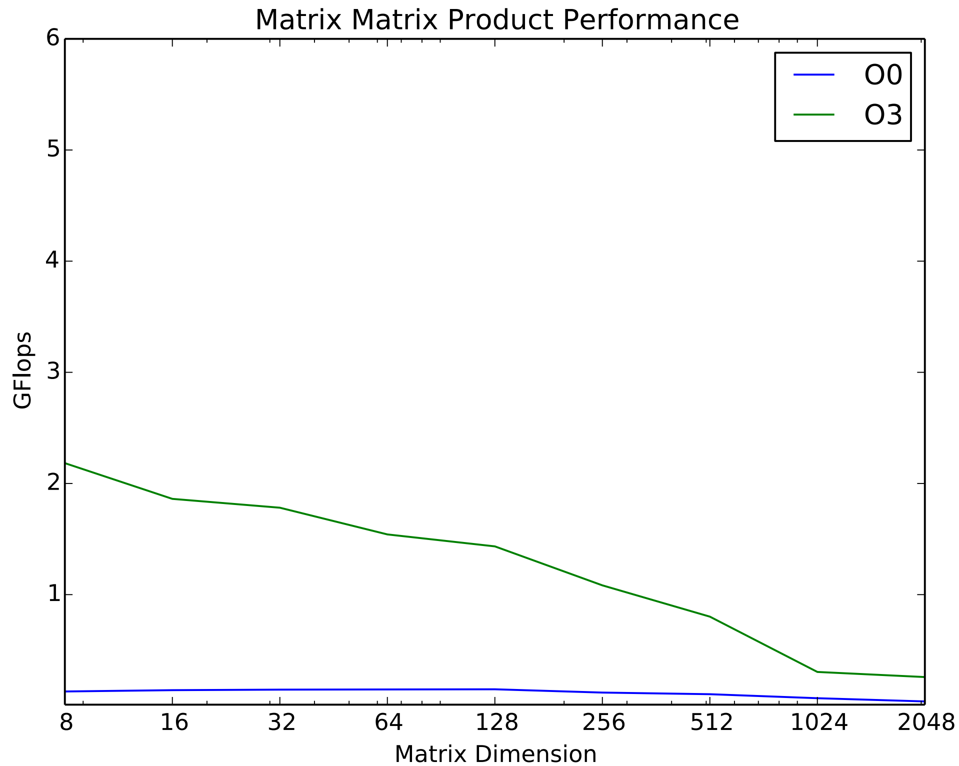
```
Matrix operator*(const Matrix& A, const Matrix&B) {
  Matrix C(A.num_rows(), B.num_cols());
  multiply(A, B, C);
  return C;
}

void multiply(const Matrix& A, const Matrix&B, Matrix&C) {
  for (size_t i = 0; i < A.num_rows(); ++i) {
    for (size_t j = 0; j < B.num_cols(); ++j) {
      for (size_t k = 0; k < A.num_cols(); ++k) {
        C(i,j) += A(i,k) * B(k,j);
      }
    }
  }
}
```

C++ Core Guideline Violation

F.20: For "out" output values, prefer return values to output parameters

# Base Performance Results



# The Three Most Important Requirements for HPC

- Locality
- Locality
- Locality

# Improving Locality

```
void multiply(const Matrix& A, const Matrix&B, Matrix&C) {
  for (size_t i = 0; i < A.num_rows(); ++i) {
    for (size_t j = 0; j < B.num_cols(); ++j) {
      for (size_ k = 0; k < A.num_cols(); ++k) {
        C(i,j) += A(i,k) * B(k,j);
      }
    }
  }
}
```

What can be reused?

- Load `C(i,j)` into register
- Load `A(i,k)` into register
- Load `B(k,j)` into register
- Multiply
- Add
- Store `C(i,j)`

- Four memory operations and two floating point operations per iteration
- 2/6 = 1/3 flop per cycle (if each operation is one cycle)

# Hoisting

Hoist C(i,j)

Why not automatically?

- Load `A(i,k)`
- Load `B(k,j)`
- Multiply
- Add

```
void multiply(const Matrix& A, const Matrix&B, Matrix&C) {
  for (size_t i = 0; i < A.num_rows(); ++i) {
    for (size_t j = 0; j < B.num_cols(); ++j) {
      double t = C(i,j);
      for (size_t k = 0; k < A.num_cols(); ++k) {
        t += A(i,k) * B(k,j);
      }
      C(i,j) = t;
    }
  }
```

- Two memory operations and two floating point operations per iteration
- 2/4 = 1/2 flop per cycle (if each operation is one cycle)

# Improving Locality: Unroll and Jam

```
void tiledMultiply2x2(const Matrix& A, const Matrix&B
  for (size_t i = 0; i < A.num_rows(); i += 2) {
    for (size_t j = 0; j < B.num_cols(); j += 2) {
      for (size_t k = 0; k < A.num_cols(); ++k) {
            C(i  , j  ) += A(i  , k) * B(k, j  );
            C(i  , j+1) += A(i  , k) * B(k, j+1);
            C(i+1, j  ) += A(i+1, k) * B(k, j  );
            C(i+1, j+1) += A(i+1, k) * B(k, j+1);
      }
    }
  }
}
```

B(k,j) is used twice

B(k,j+1) is used twice

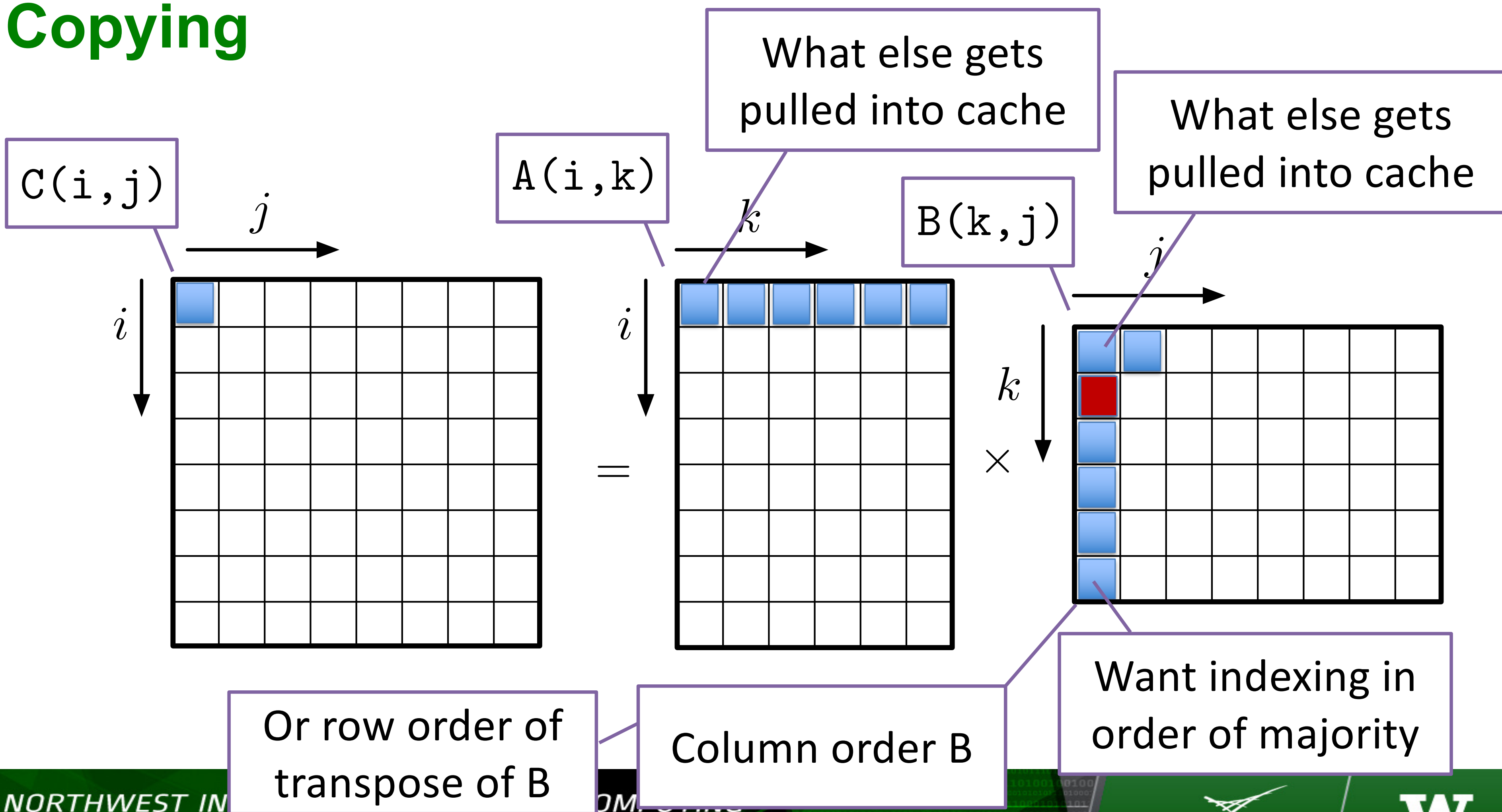
A(i,k) is used twice

A(i+1,k) is used twice

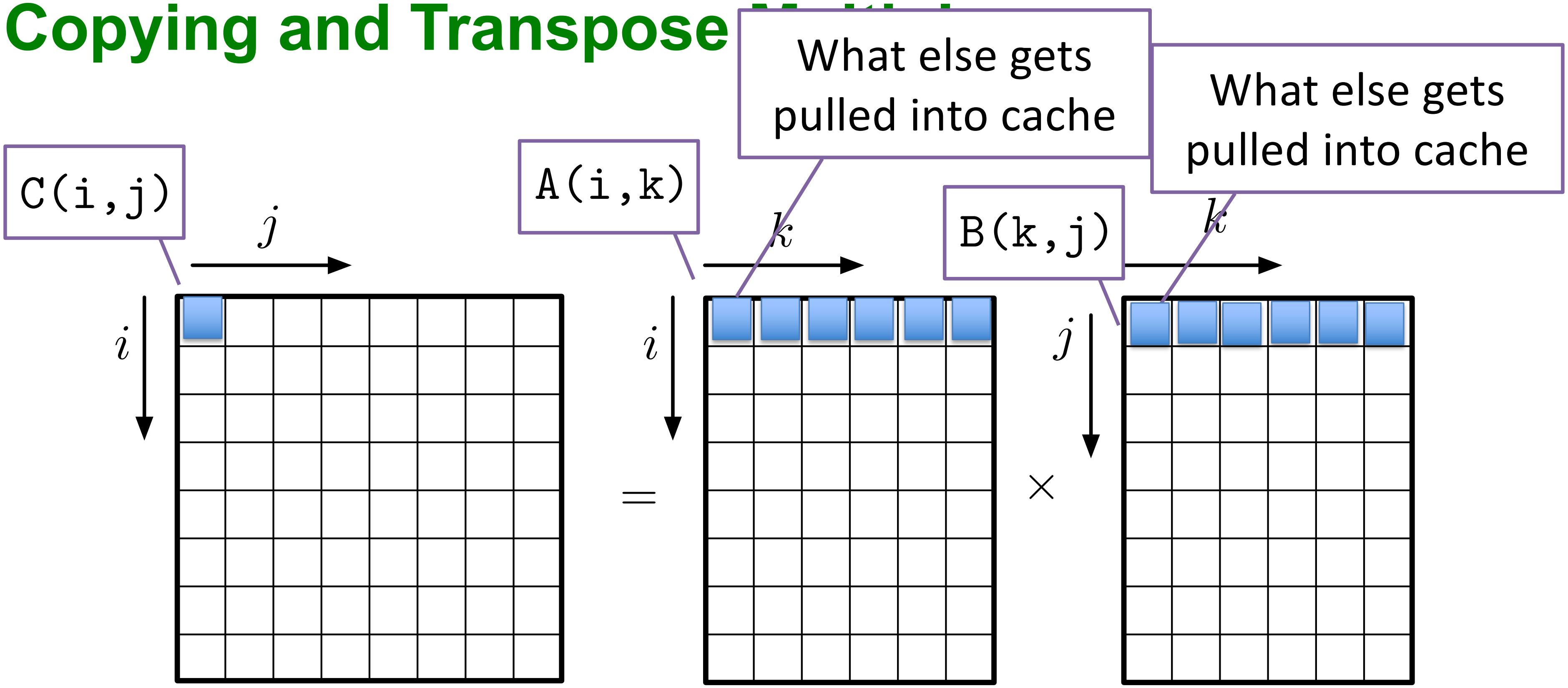
Can also hoist (independent of k)

- Four memory operations and eight floating point operations per iteration
- 8/12 = 2/3 flop per cycle (if each operation is one cycle) – 2X the base case

# Copying


C(i,j)
A(i,k)
B(k,j)
What else gets pulled into cache
What else gets pulled into cache
j
i
k
i
j
k
=
×
Or row order of transpose of B
Column order B
Want indexing in order of majority

# Copying and Transpose

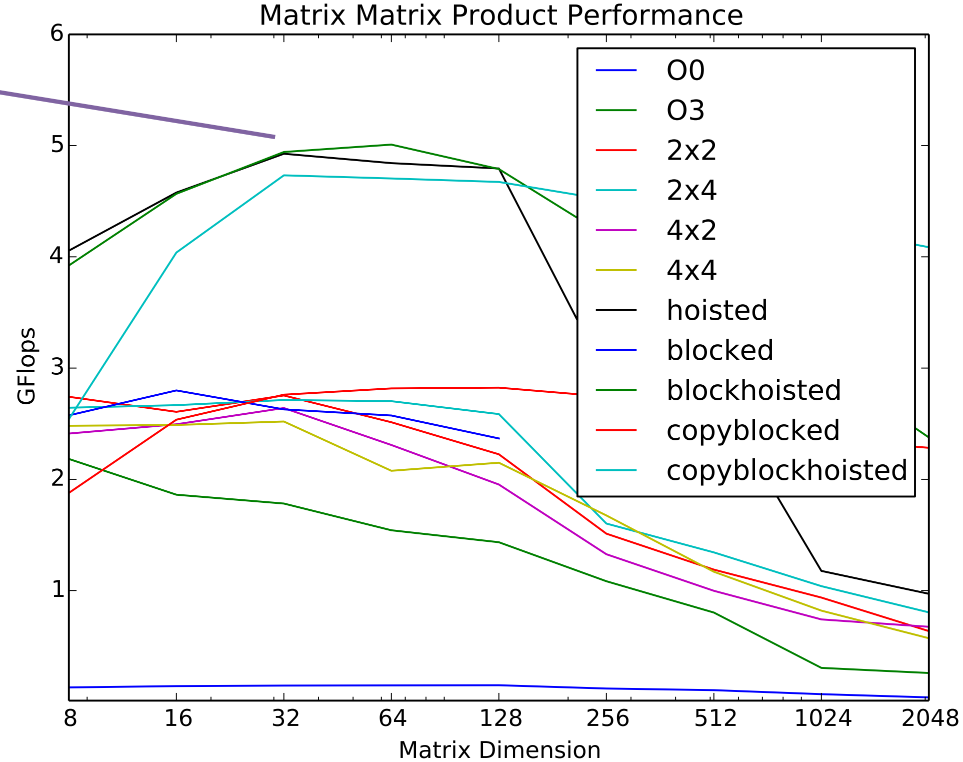


# Blocking and Tiling and Hoisting and Copying

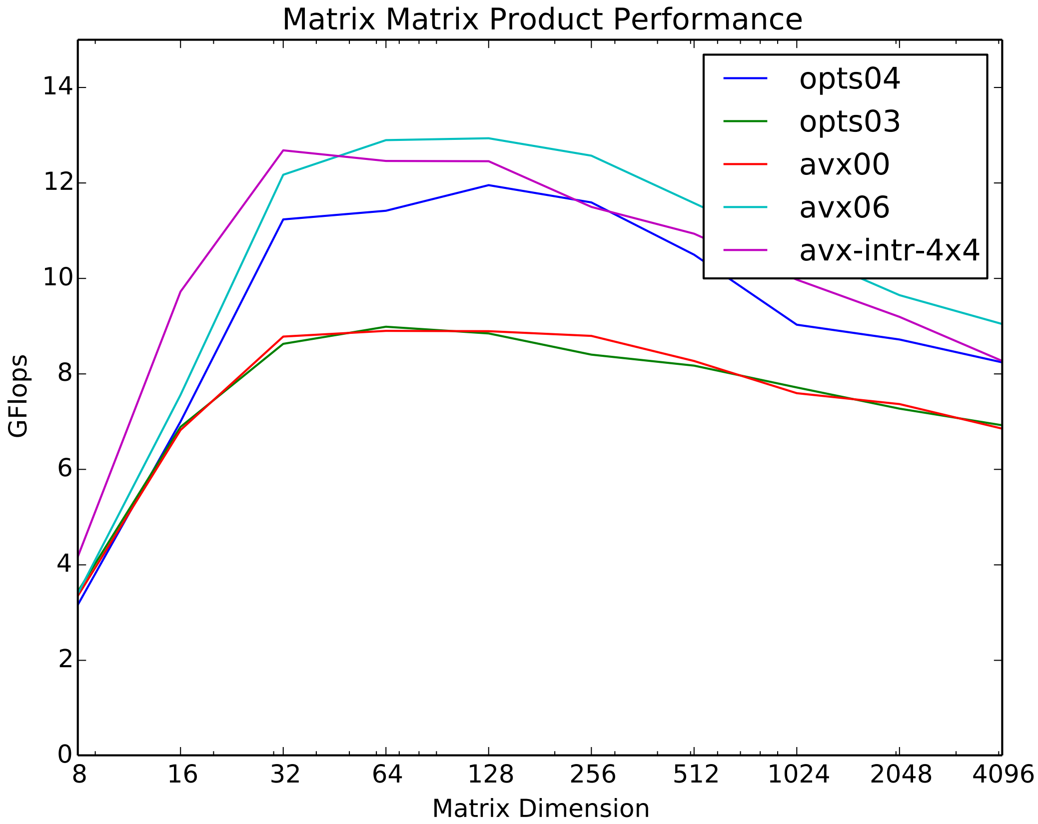
Is this the best we can do?

How good is it anyway?

(cf PS 4A)



# Writing Faster Matrix Matrix Product



# Under the Hood

```
for (int i = ii; i < ii+blocksize; i += 4) {
  for (int j = jj, jb = 0; j < jj+blocksize; j += 4, jb += 4) {

    __m256d t0x = _mm256_load_pd(&C(i,  j));
    __m256d t1x = _mm256_load_pd(&C(i+1,j));
    __m256d t2x = _mm256_load_pd(&C(i+2,j));
    __m256d t3x = _mm256_load_pd(&C(i+3,j));

    for (int k = kk, kb = 0; k < kk+blocksize; ++k, ++kb) {

     __m256d bx = _mm256_setr_pd(BB(jb,kb), BB(jb+1,kb), BB(jb+2,kb), BB(jb+3,kb));

     __m256d a0 = _mm256_broadcast_sd(&A(i  ,k));
      a0  = _mm256_mul_pd(bx,  a0);
      t0x = _mm256_add_pd(t0x, a0);

      __m256d a1 = _mm256_broadcast_sd(&A(i+1,k));
      a1  = _mm256_mul_pd(bx,  a1);
      t1x = _mm256_add_pd(t1x, a1);

      __m256d a2 = _mm256_broadcast_sd(&A(i+2,k));
      a2  = _mm256_mul_pd(bx,  a2);
      t2x = _mm256_add_pd(t2x, a2);

      __m256d a3 = _mm256_broadcast_sd(&A(i+3,k));
      a3  = _mm256_mul_pd(bx,  a3);
      t3x = _mm256_add_pd(t3x, a3);
    }

    _mm256_store_pd(&C(i,  j), t0x);
    _mm256_store_pd(&C(i+1,j), t1x);
    _mm256_store_pd(&C(i+2,j), t2x);
    _mm256_store_pd(&C(i+3,j), t3x);
  }
}
```

```
vbroadcastsd    (%rdx,%r8,8), %ymm3
vfmadd213pd     %ymm4, %ymm8, %ymm3
vbroadcastsd    (%rsi,%r8,8), %ymm2
vfmadd213pd     %ymm5, %ymm8, %ymm2
vbroadcastsd    (%rbx,%r8,8), %ymm1
vfmadd213pd     %ymm6, %ymm8, %ymm1
vbroadcastsd    (%rdi,%r8,8), %ymm0
vfmadd213pd     %ymm7, %ymm8, %ymm0
```

X86 Assembly

AVX instructions

256 bit register

Fused Multiply-Add

Multiply-Add are separate here

8 FLOPS per cycle?

# Vector Operations from C++

```
for (int i = ii; i < ii+blocksize; i += 2) {
  for (int j = jj, jb = 0; j < jj+blocksize; j += 2, jb += 2) {
    double t00 = C(i,j);       double t01 = C(i,j+1);
    double t10 = C(i+1,j);     double t11 = C(i+1,j+1);

    for (int k = kk, kb = 0; k < kk+blocksize; ++k, ++kb) {
      t00 += A(i  , k) * BB(jb  , kb);
      t01 += A(i  , k) * BB(jb+1, kb);
      t10 += A(i+1, k) * BB(jb  , kb);
      t11 += A(i+1, k) * BB(jb+1, kb);
    }

    C(i,  j) = t00;  C(i,  j+1) = t01;
    C(i+1,j) = t10;  C(i+1,j+1) = t11;
  }
}
```

```
vmovupd          (%r8,%r13,8), %ymm4
vmovupd          (%r11,%r13,8), %ymm5
vfmadd231pd      %ymm4, %ymm5, %ymm3
vmovupd -32      (%r9,%r13,8), %ymm6
vfmadd231pd      %ymm4, %ymm6, %ymm2
vmovupd          (%rdx,%r13,8), %ymm4
vfmadd231pd      %ymm5, %ymm4, %ymm1
vfmadd231pd      %ymm6, %ymm4, %ymm0
vmovupd          (%rcx,%r13,8), %ymm4
vmovupd 32       (%r11,%r13,8), %ymm5
vfmadd231pd      %ymm4, %ymm5, %ymm3
vmovupd          (%r9,%r13,8), %ymm6
vfmadd231pd      %ymm4, %ymm6, %ymm2
vmovupd          (%rbx,%r13,8), %ymm4
vfmadd231pd      %ymm5, %ymm4, %ymm1
vfmadd231pd      %ymm6, %ymm4, %ymm0
```

Fused Multiply-Add

256 bit registers

# LLVM

# Compiler Optimizations

```
$ echo 'int;' | $(CXX) -xc++ $(CXXFLAGS) - -o /dev/null -\#\#\#
```

- Many options
- -Ofast
- -march=native

```
lums658@WE31821=> make optreport
echo 'int;' | c++ -xc -Ofast -march=native -DNDEBUG -fslp-vectorize-aggressive -mxsave -mavx -ma
vx2  -std=c++14 -Wc++14-extensions -fslp-vectorize-aggressive -mxsave -mavx -mavx2 -Wall - -o /d
ev/null -\#\#\#
Apple LLVM version 8.1.0 (clang-802.0.41)
Target: x86_64-apple-darwin16.5.0
Thread model: posix
InstalledDir: /Applications/Xcode.app/Contents/Developer/Toolchains/XcodeDefault.xctoolchain/usr
/bin
 "/Applications/Xcode.app/Contents/Developer/Toolchains/XcodeDefault.xctoolchain/usr/bin/clang"
"-cc1" "-triple" "x86_64-apple-macosx10.12.0" "-Wdeprecated-objc-isa-usage" "-Werror=deprecated-
objc-isa-usage" "-emit-obj" "-disable-free" "-disable-llvm-verifier" "-discard-value-names" "-ma
in-file-name" "-" "-mrelocation-model" "pic" "-pic-level" "2" "-mthread-model" "posix" "-mdisabl
e-fp-elim" "-menable-no-infs" "-menable-no-nans" "-menable-unsafe-fp-math" "-fno-signed-zeros" "
-freciprocal-math" "-ffp-contract=fast" "-ffast-math" "-masm-verbose" "-munwind-tables" "-target
-cpu" "haswell" "-target-feature" "+sse2" "-target-feature" "+cx16" "-target-feature" "-tbm" "-t
arget-feature" "-avx512ifma" "-target-feature" "-avx512dq" "-target-feature" "-fma4" "-target-fe
ature" "-prfchw" "-target-feature" "+bmi2" "-target-feature" "-xsavec" "-target-feature" "+fsgsb
ase" "-target-feature" "+popcnt" "-target-feature" "+aes" "-target-feature" "-pcommit" "-target-
feature" "-xsaves" "-target-feature" "-avx512er" "-target-feature" "-clwb" "-target-feature" "-a
vx512f" "-target-feature" "-pku" "-target-feature" "-smap" "-target-feature" "+mmx" "-target-fea
ture" "-xop" "-target-feature" "-rdseed" "-target-feature" "-hle" "-target-feature" "-sse4a" "-t
arget-feature" "-avx512bw" "-target-feature" "-clflushopt" "-target-feature" "-avx512vl" "-targe
t-feature" "+invpcid" "-target-feature" "-avx512cd" "-target-feature" "-rtm" "-target-feature" "
+fma" "-target-feature" "+bmi" "-target-feature" "-mwaitx" "-target-feature" "+rdrnd" "-target-f
eature" "+sse4.1" "-target-feature" "+sse4.2" "-target-feature" "+sse" "-target-feature" "+lzcnt
" "-target-feature" "+pclmul" "-target-feature" "-prefetchwt1" "-target-feature" "+f16c" "-targe
t-feature" "+ssse3" "-target-feature" "-sgx" "-target-feature" "+cmov" "-target-feature" "-avx51
2vbmi" "-target-feature" "+movbe" "-target-feature" "+xsaveopt" "-target-feature" "-sha" "-targe
t-feature" "-adx" "-target-feature" "-avx512pf" "-target-feature" "+sse3" "-target-feature" "+xs
ave" "-target-feature" "+avx" "-target-feature" "+avx2" "-target-linker-version" "278.4" "-dwarf
-column-info" "-debugger-tuning=lldb" "-resource-dir" "/Applications/Xcode.app/Contents/Develope
r/Toolchains/XcodeDefault.xctoolchain/usr/bin/../lib/clang/8.1.0" "-D" "NDEBUG" "-Ofast" "-Wc++1
4-extensions" "-Wall" "-std=c++14" "-fdebug-compilation-dir" "/Users/lums658/git/amath-583/src"
"-ferror-limit" "19" "-fmessage-length" "96" "-stack-protector" "1" "-fblocks" "-fobjc-runtime=m
acosx-10.12.0" "-fencode-extended-block-signature" "-fmax-type-align=16" "-fdiagnostics-show-opt
ion" "-fcolor-diagnostics" "-vectorize-loops" "-vectorize-slp" "-vectorize-slp-aggressive" "-o"
"/var/folders/4z/vn0681g52rx8b18_q2r1fcv0lzfm0s/T/--7075ee.o" "-x" "c" "-"
 "/Applications/Xcode.app/Contents/Developer/Toolchains/XcodeDefault.xctoolchain/usr/bin/ld" "-d
emangle" "-lto_library" "/Applications/Xcode.app/Contents/Developer/Toolchains/XcodeDefault.xcto
olchain/usr/lib/libLTO.dylib" "-dynamic" "-arch" "x86_64" "-macosx_version_min" "10.12.0" "-o" "
/dev/null" "/var/folders/4z/vn0681g52rx8b18_q2r1fcv0lzfm0s/T/--7075ee.o" "-lc++" "-lSystem" "/Ap
plications/Xcode.app/Contents/Developer/Toolchains/XcodeDefault.xctoolchain/usr/bin/../lib/clang
/8.1.0/lib/darwin/libclang_rt.osx.a"
```

# Compiler Diagnostics

- There are some flags to see what the compiler is doing

```
optflags          :
                  echo 'int;' | $(CXX) -xc++ $(CXXFLAGS) - -o /dev/null -\#\#\#

defreport         :
                  $(CXX) -dM -E -x c++ /dev/null

Matrix.o .        :
                  $(CXX) -c $(CXXFLAGS) -Rpass=.* -o Matrix.o
```

Print flags passed to compiler

Print internal #defines

Print what optimizations are applied (and where)

# Internal #define

defreport :

```
$(CXX) -dM -E -x c++ /dev/null
```

```
#define OBJC_NEW_PROPERTIES 1
#define _LP64 1
#define __APPLE_CC__ 6000
#define __APPLE__ 1
#define __ATOMIC_ACQUIRE 2
#define __ATOMIC_ACQ_REL 4
#define __ATOMIC_CONSUME 1
#define __ATOMIC_RELAXED 0
#define __ATOMIC_RELEASE 3
#define __ATOMIC_SEQ_CST 5
#define __BLOCKS__ 1
#define __CHAR16_TYPE__ unsigned short
#define __CHAR32_TYPE__ unsigned int
```

340+ total

Very useful for conditional compilation

```
#ifdef __AVX__
    __m128d a = _mm256_extractf128_pd(tx, 0);
    __m128d b = _mm256_extractf128_pd(tx, 1);
    _mm_store_pd(&C(i,j)    , a);
    _mm_store_pd(&C(i+1, j), b);
#endif // __AVX__
```

# Optimization Report

```
Matrix.o          :
                    $(CXX) -c $(CXXFLAGS) -Rpass=.* -o Matrix.o
```

```
Matrix.cpp: 52: 7: remark: vectorized loop (vectorization width: 4, interleaved count: 4) [-
      for (int k = 0; k < A.numCols(); ++k) {
      ^
Matrix.cpp: 52: 7: remark: unrolled loop by a factor of 2 with run-time trip count [-Rpass=]
Matrix.cpp: 50: 5: remark: unrolled loop by a factor of 8 with run-time trip count [-Rpass=]
    for (int j = 0; j < B.numCols(); ++j) {
```

```
for (int j = 0; j < B.numCols(); ++j) {
  double t = C(i,j);
  for (int k = 0; k < A.numCols(); ++k) {
    t += A(i,k) * B(k,j);
  }
  C(i,j) = t;
}
```

Selects all

Unroll
Vectorization
Inline

# As a Last Resort

```
%.s          : %.cpp
               $(CXX) -S $(CXXFLAGS) $<
```

Matrix.s.opt.05

```
                                        ##          Parent Loop BB11_25 Depth=4
                                        ##            Parent Loop BB11_26 Depth=5
                                        ## =>           This Inner Loop Header:
Depth=6
        vmovupd         (%r8,%r13,8), %ymm4
        vmovupd         (%r11,%r13,8), %ymm5
        vfmadd231pd     %ymm4, %ymm5, %ymm3
        vmovupd         -32(%r9,%r13,8), %ymm6
        vfmadd231pd     %ymm4, %ymm6, %ymm2
        vmovupd         (%rdx,%r13,8), %ymm4
        vfmadd231pd     %ymm5, %ymm4, %ymm1
        vfmadd231pd     %ymm6, %ymm4, %ymm0
        vmovupd         (%rcx,%r13,8), %ymm4
        vmovupd         32(%r11,%r13,8), %ymm5
        vfmadd231pd     %ymm4, %ymm5, %ymm3
        vmovupd         (%r9,%r13,8), %ymm6
        vfmadd231pd     %ymm4, %ymm6, %ymm2
        vmovupd         (%rbx,%r13,8), %ymm4
        vfmadd231pd     %ymm5, %ymm4, %ymm1
        vfmadd231pd     %ymm6, %ymm4, %ymm0
        addq            $8, %r13
        cmpq            %r13, %rsi
        jne     LBB11_39
LBB11_40:                               ##   in Loop: Header=BB11_26 Depth=5
-:**-  Matrix.s.opt.05   32% (3043,0)  (Assembler WordWrap) Wed Apr 19 8:04AM 1.45
```

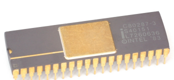
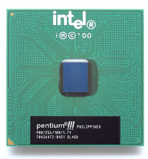
# Advanced Vector Extensions

SIMD?

Multi Media Extensions

Streaming SIMD Extensions

Advanced Vector Extensions

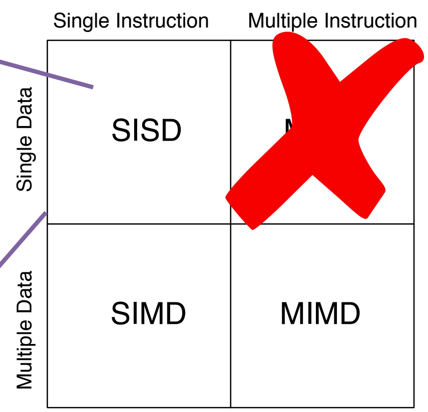
| 1980 | 1997 | 1999 | 2001 | 2004<br>2006<br>2007<br>2008 | 2011 | 2013 | 2016 |
|---|---|---|---|---|---|---|---|
| 8087 | MMX | SSE | SSE2 | SSE3<br>SSE3.1<br>SSE4.1<br>SSE4.2 | AVX | AVX2 | AVX512 |
|  |  |  |  | |  |  | |
| 8 80-bit stack registers | 8 64-bit registers | 8 128-bit registers (single) (xmm) | 8 128-bit registers (double) | Many new instructions | 16 256-bit registers (ymm) | | 32 512-bit registers (zmm) |

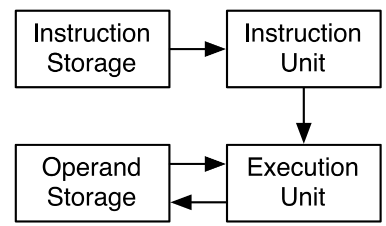
# Flynn's Taxonomy (Aside)

Anyone in HPC must know Flynn's taxonomy

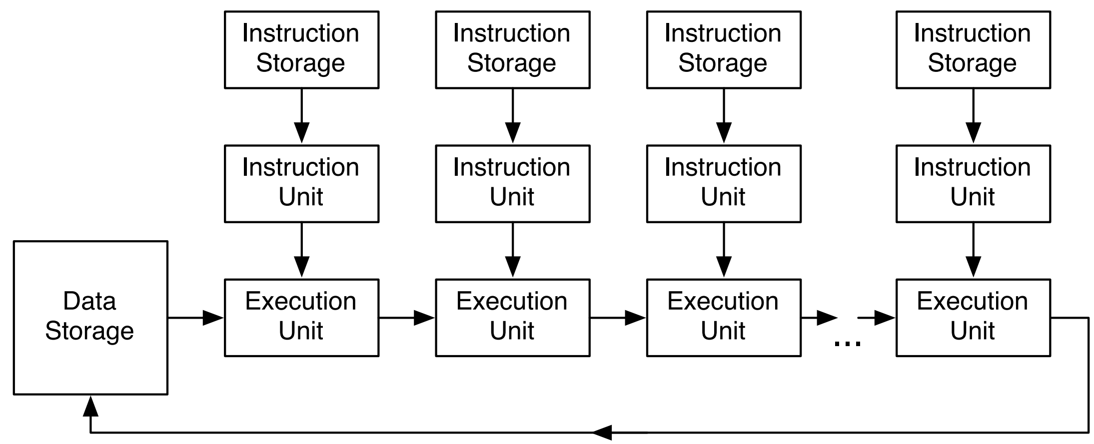
- **Classic** classification of parallel architectures (Michael Flynn, 1966)

Plain old sequential



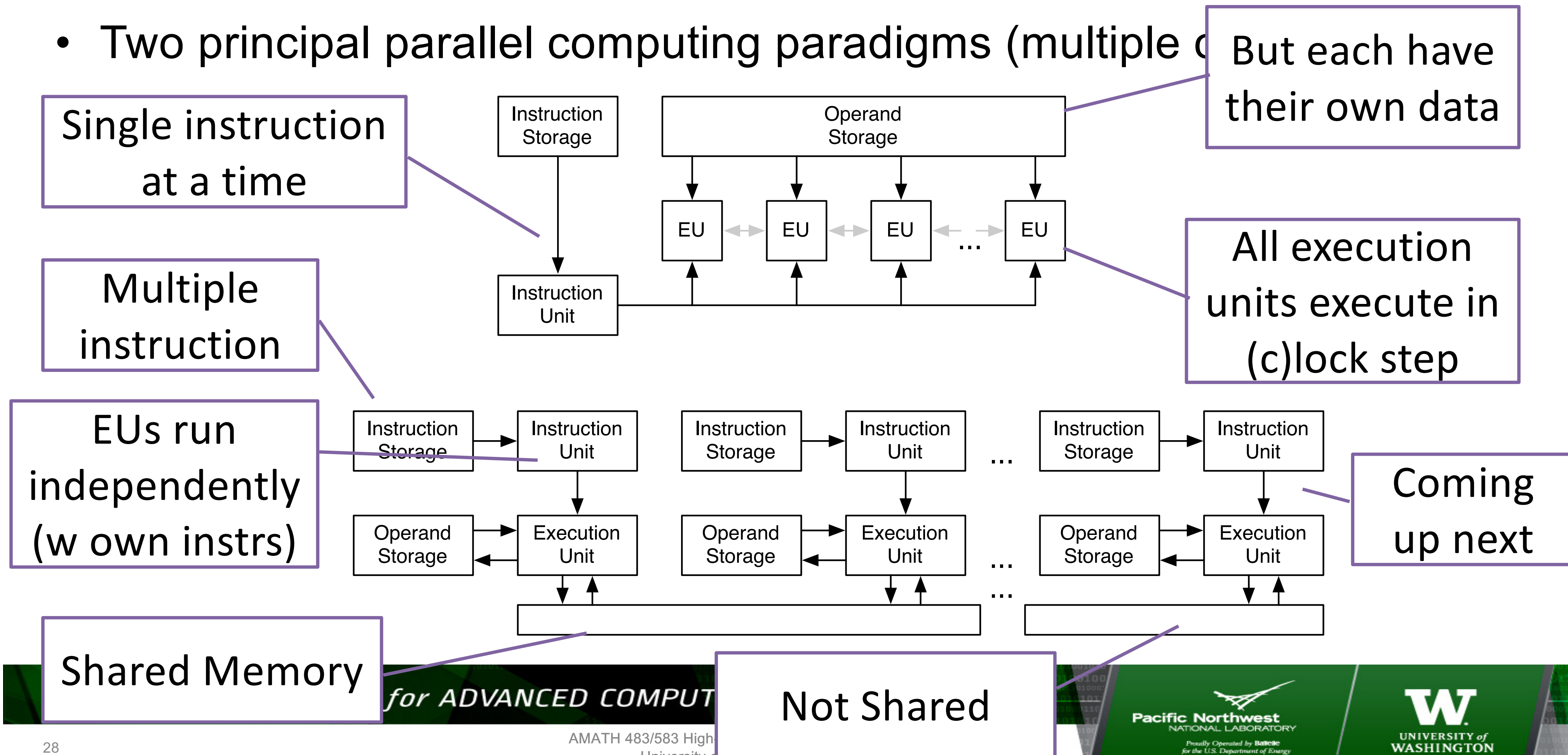




Based on multiplicity of instruction streams, data storage



# SIMD and MIMD

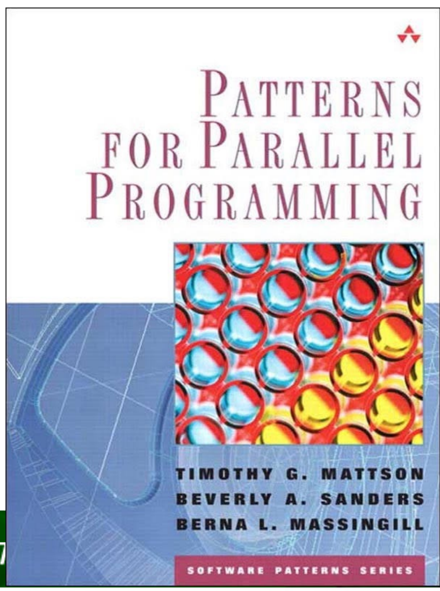
- Two principal parallel computing paradigms (multiple c

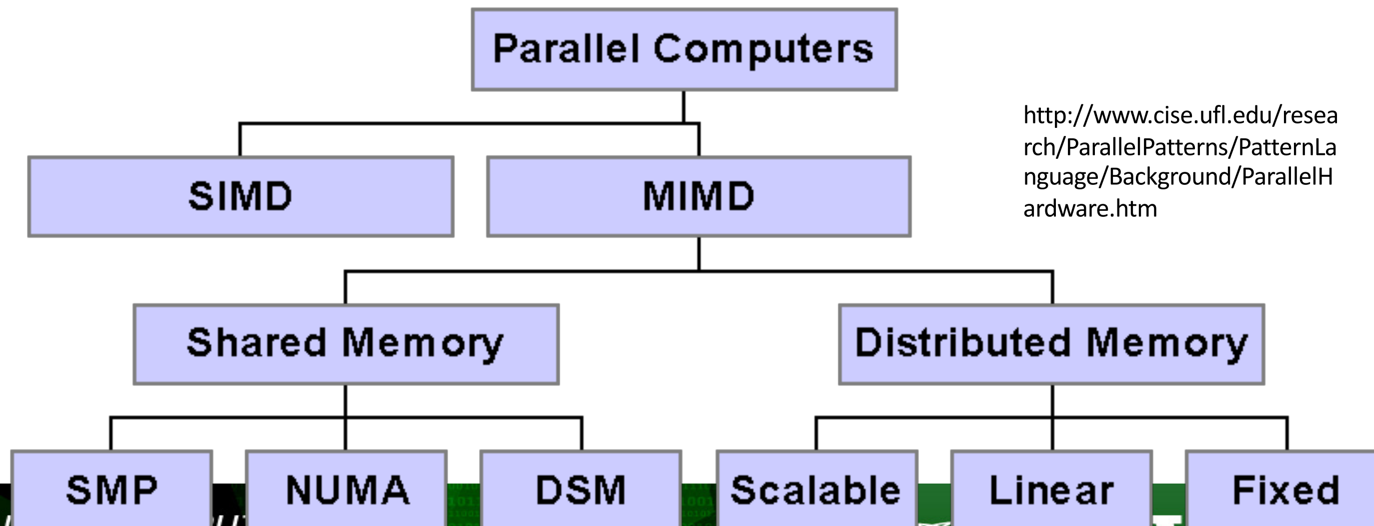


# A More Refined (Programmer-Oriented) Taxonomy

- Three major mod … uted Memory
- Different program … sociated with different modes c … MPI for distributed)
- A modern supercomputer will have all three major modes present

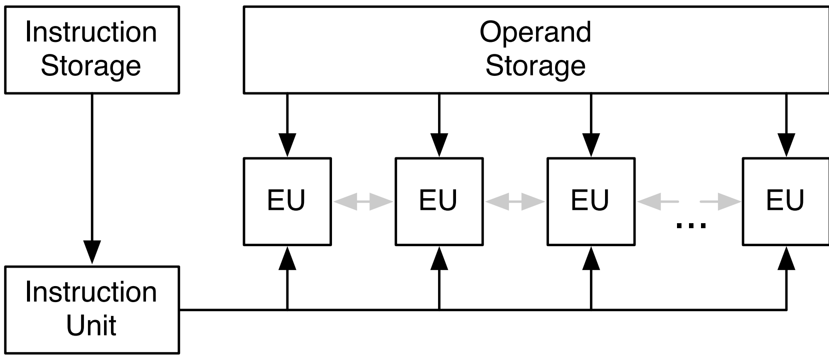
**We will come back to this soon**




http://www.cise.ufl.edu/research/ParallelPatterns/PatternLanguage/Background/ParallelHardware.htm

# SIMD in SSE/AVX

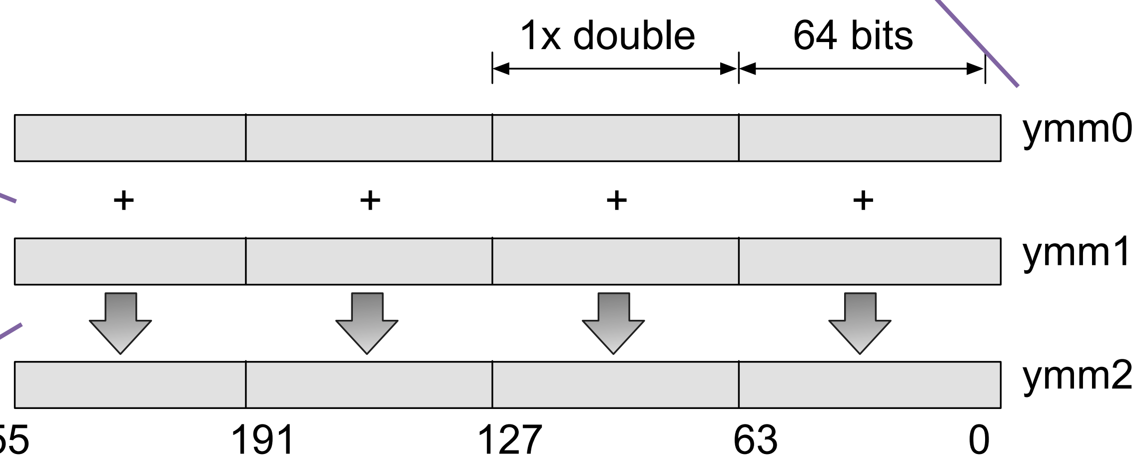



Flynn's original conceptual model

ymm are 256 bit registers

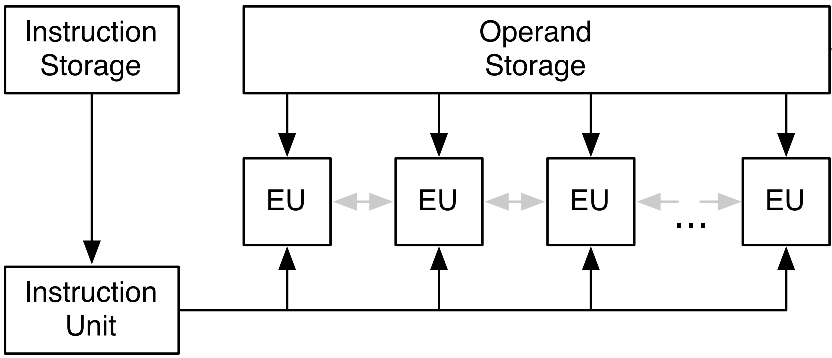
```
vfadd231pd  %ymm0, %ymm1, %ymm2
```

One machine instruction




Adds all four doubles ***simultaneously***

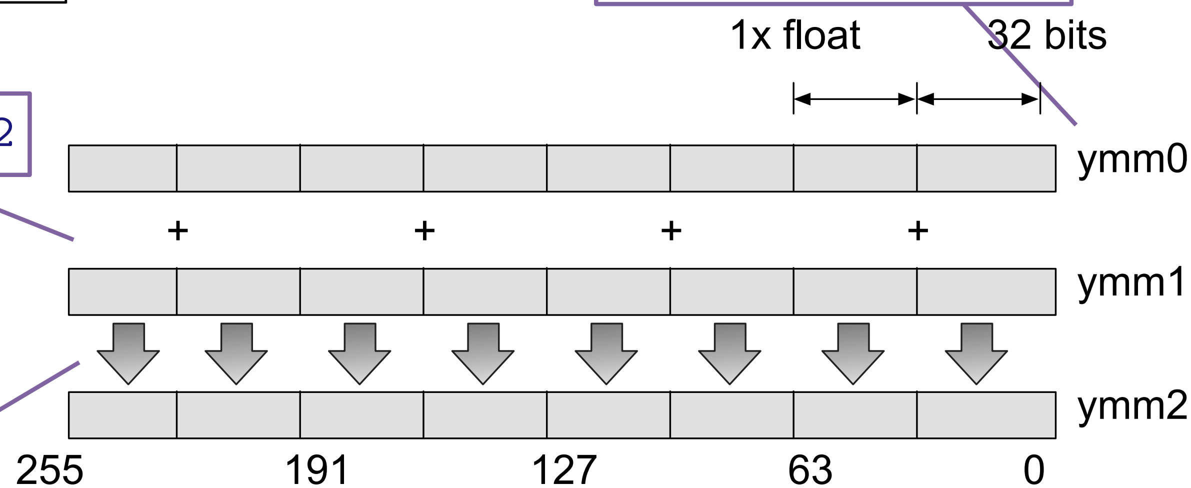
# SIMD in SSE/AVX




Flynn's original conceptual model

ymm are 256 bit registers

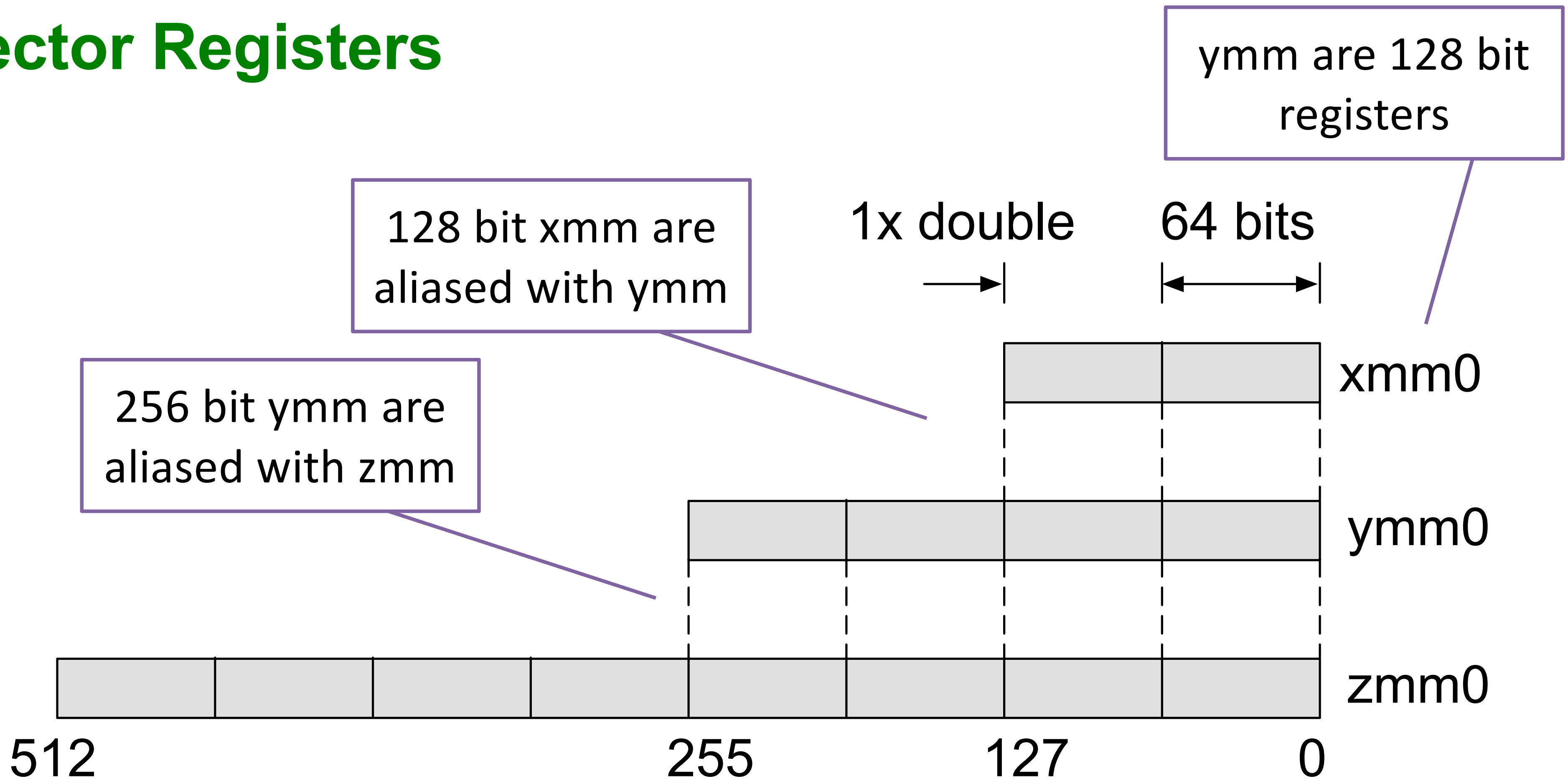
`vfadd231ps %ymm0, %ymm1, %ymm2`



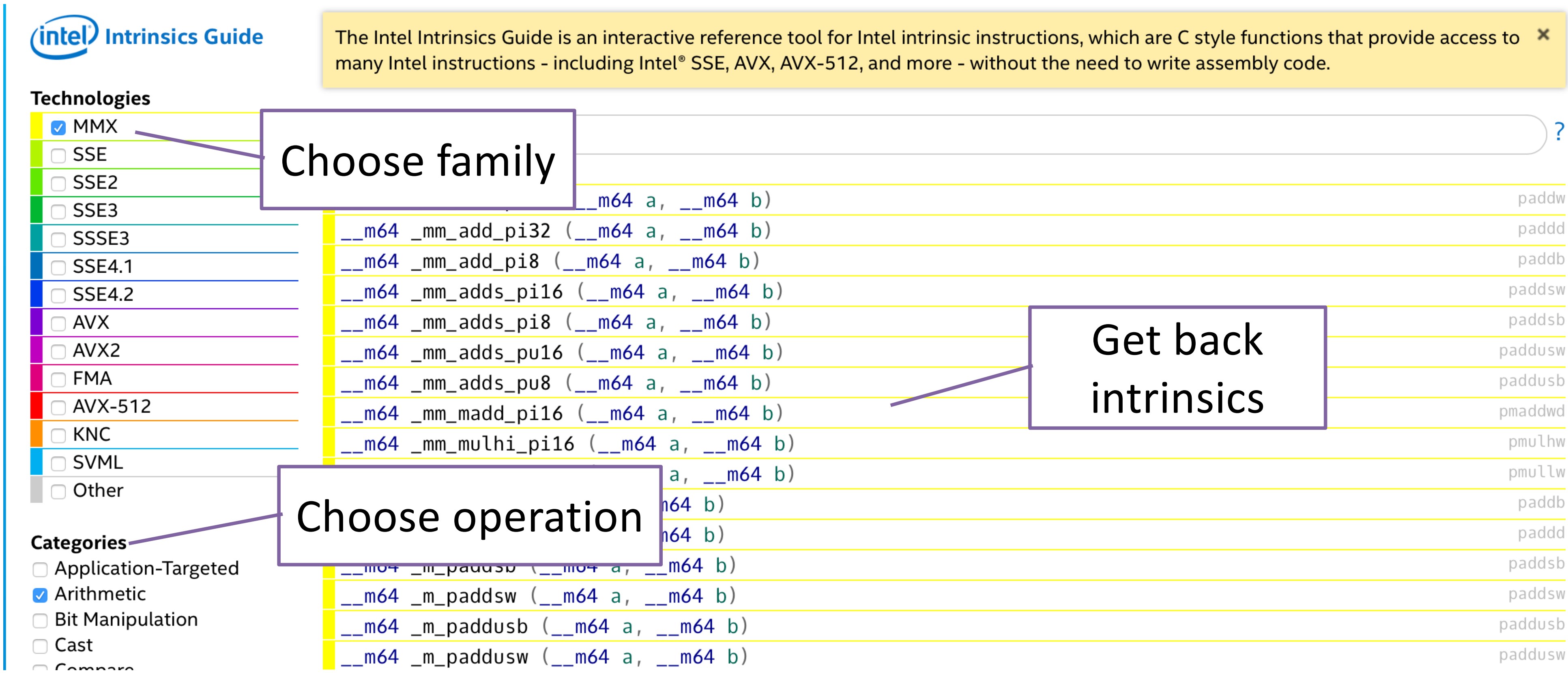

One machine instruction

Adds all eight floats ***simultaneously***

# Vector Registers



# Intel Intrinsics Guide



# Intrinsics

```
__m512d _mm512_fnmadd_pd (__m512d a, __m512d b, __m512d c)
```

vfnmadd132pd, vfnmadd213pd, vfnmadd231pd

**Synopsis**

```
__m512d _mm512_fnmadd_pd (__m512d a, __m512d b, __m512d c)
#include "immintrin.h"
Instruction: vfnmadd132pd zmm {k}, zmm, zmm
             vfnmadd213pd zmm {k}, zmm, zmm
             vfnmadd231pd zmm {k}, zmm, zmm
CPUID Flags: AVX512F for AVX-512, KNCNI for KNC
```

How to access AVX instructions from C/C++

The machine instruction(s) that is/are generated

**Description**

Multiply packed double-precision (64-bit) floating-point elements in a and [...] c, and store the results in dst.

**Operation**

```
FOR j := 0 to 7
	i := j*64
	dst[i+63:i] := -(a[i+63:i] * b[i+63:i]) + c[i+63:i]
ENDFOR
dst[MAX:512] := 0
```

Does your CPU support this instruction?

**Performance**

| Architecture | Latency | Throughput |
|---|---|---|
| Knights Landing | 6 | 0.5 |

# CPU ID

- The cpuid machine instruction can be used to query the CPU about what features it supports

```
$ docker run amath583/cpuinfo
This CPU supports CPUID_EAX_CORE2_DUO_8K
This CPU supports CPUID_EBX_AVX2
This CPU supports CPUID_ECX_SSE3
This CPU supports CPUID_ECX_SSSE3
This CPU supports CPUID_ECX_FMA
This CPU supports CPUID_ECX_SSE41
This CPU supports CPUID_ECX_SSE42
This CPU supports CPUID_ECX_AES
This CPU supports CPUID_ECX_AVX
This CPU supports CPUID_ECX_F16C
This CPU supports CPUID_ECX_HYPERVISOR
```

Processor family

Supported features

Under docker the cpu will be in hypervisor mode

# Issuing ASM directly

```
int input = 0, output = 0;

__asm__("cpuid;"
        :"=a"(output)
        :"a"(input)
        :"%ebx","%ecx","%edx");  // clobbered registers
```

C++ variables

cpuid instruction

The register EAX is mapped to variable “output” on completion

The variable “input” is mapped to register EAX at start

Preserve these registers

# What Does the Compiler Look for?

```
void basicMultiply(const Matrix& A, const Matrix&B, Matrix&C) {
  for (int i = 0; i < A.numRows(); ++i) {
    for (int j = 0; j < B.numCols(); ++j) {
      for (int k = 0; k < A.numCols(); ++k) {
        C(i,j) += A(i,k) * B(k,j);
      }
    }
  }
}
```

```
Matrix.cpp:31:7: remark: unrolled loop by a factor of 4 \
    with run-time trip count [-Rpass=loop-unroll]

      for (int k = 0; k < A.numCols(); ++k) {
```

# Unrolling

```
void basicMultiply(const Matrix& A, const Matrix&B, Matrix&C) {
  for (int i = 0; i < A.numRows(); ++i) {
    for (int j = 0; j < B.numCols(); ++j) {
      for (int k = 0; k < A.numCols(); k += 4) {
        C(i,j) += A(i, k + 0) * B(k + 0, j);
        C(i,j) += A(i, k + 1) * B(k + 1, j);
        C(i,j) += A(i, k + 2) * B(k + 2, j);
        C(i,j) += A(i, k + 3) * B(k + 3, j);
      }
    }
  }
}
```

# Generated Code

```
vmovsd      (%rdi,%r11,8), %xmm1
vmulsd      -8(%r13), %xmm1, %xmm1
vaddsd      %xmm1, %xmm0, %xmm0
vmovsd      %xmm0, (%rdx,%r14,8)
vmovsd      (%r10,%rdi), %xmm1
vmulsd      (%r13), %xmm1, %xmm1
vaddsd      %xmm1, %xmm0, %xmm0
vmovsd      %xmm0, (%rdx,%r14,8)
```

# What Does the Compiler Look for?

```
void hoistedMultiply(const Matrix& A, const Matrix&B, Matrix&C) {
  for (int i = 0; i < A.numRows(); ++i) {
    for (int j = 0; j < B.numCols(); ++j) {
      double t = C(i,j);
      for (int k = 0; k < A.numCols(); ++k) {
        t += A(i,k) * B(k,j);
      }
      C(i,j) = t;
    }
  }
}
```

```
Matrix.cpp:52:7: remark: vectorized loop \
    (vectorization width: 4, interleaved count: 4) [-Rpass=

      for (int k = 0; k < A.numCols(); ++k) {
      ^
Matrix.cpp:52:7: remark: unrolled loop by a factor of 2 \
    with run-time trip count [-Rpass=loop-unroll]
Matrix.cpp:50:5: remark: unrolled loop by a factor of 8 \
    with run-time trip count [-Rpass=loop-unroll]

    for (int j = 0; j < B.numCols(); ++j) {
    ^
```

# What Does the Compiler Look for?

```
./Matrix.hpp:26:69: remark: _ZNKSt3__16vectorIdNS_9allocatorIdEEEixEm inlined into
      _ZNK6MatrixclEmm [-Rpass=inline]
  const double &operator()(size_type i, size_type j) const { return arrayData[i*jCols + j];
                                                                    ^
./Matrix.hpp:25:69: remark: _ZNSt3__16vectorIdNS_9allocatorIdEEEixEm inlined into
      _ZN6MatrixclEmm [-Rpass=inline]
        double &operator()(size_type i, size_type j)       { return arrayData[i*jCols + j];
```

Signatures get mangled

operator()() Function

Function call is replaced with body of code

Easier if body is available to compiler

i.e., if it is ***defined in the header file***

```
vmovsd    (%rdi,%r11,8), %xmm1
vmulsd    -8(%r13), %xmm1, %xmm1
vaddsd    %xmm1, %xmm0, %xmm0
vmovsd    %xmm0, (%rdx,%r14,8)
vmovsd    (%r10,%rdi), %xmm1
vmulsd    (%r13), %xmm1, %xmm1
vaddsd    %xmm1, %xmm0, %xmm0
vmovsd    %xmm0, (%rdx,%r14,8)
```

No function call!!

# Without Inlining

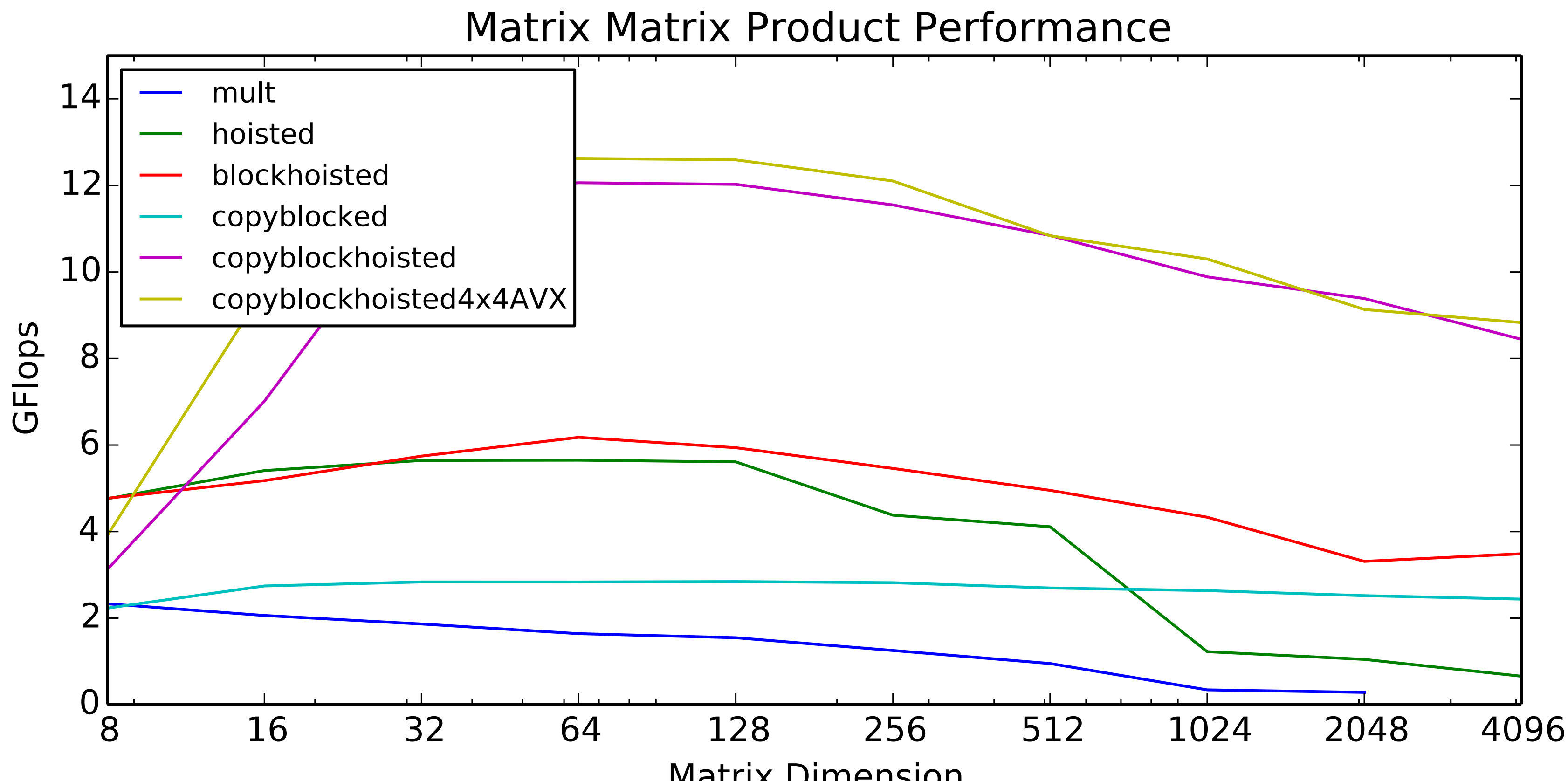
```
movq    -8(%rbp), %rdi
movslq  -28(%rbp), %rsi
movslq  -36(%rbp), %rdx
callq   __ZNK6MatrixclEmm
movsd   (%rax), %xmm0
movq    -16(%rbp), %rdi
movslq  -36(%rbp), %rsi
movslq  -32(%rbp), %rdx
movsd   %xmm0, -72(%rbp)
callq   __ZNK6MatrixclEmm
movsd   -72(%rbp), %xmm0
mulsd   (%rax), %xmm0
movq    -24(%rbp), %rdi
movslq  -28(%rbp), %rsi
movslq  -32(%rbp), %rdx
movsd   %xmm0, -80(%rbp)
callq   __ZN6MatrixclEmm
movsd   -80(%rbp), %xmm0
addsd   (%rax), %xmm0
movsd   %xmm0, (%rax)
```

operator()() function call

operator()() function call

operator()() function call

# Summary


Matrix Matrix Product Performance
mult
hoisted
blockhoisted
copyblocked
copyblockhoisted
copyblockhoisted4x4AVX
GFlops
0
2
4
6
8
10
12
14
8
16
32
64
128
256
512
1024
2048
4096
Matrix Dimension

# Recommendations

Inlining, unrolling, vectorization

- Avoid programming in assembler
- If you can't avoid that, use intrinsics – but you will need to match the instructions to the hardware (which is not portable)
- In general, let compiler determine hardware, pick instructions, and optimize
- Check your performance against performance models
- Monitor what your compiler is doing
  - Optimization report
  - Full set of flags
  - Last resort – read the assembler

Most important is to have a mental model for the vector registers and to be aware of what is possible and how to write code to be optimizable

# Review

- High Performance = Writing software to use hardware effectively
- Hardware
  - Fast clock
  - Branch prediction, other magic on chip
  - Hierarchical memory
  - Pipelining instructions
  - Vector registers and vector instructions (”SIMD”)
- Software techniques to use all of these
- Compilers!
- Our first parallel computations

# Basic Linear Algebra Subprograms (BLAS)

- Standardized set of core / kernel algorithms for numerical linear algebra
- Fortran – but various extensions to C have been created
  - Matrix ordering and function calling disciplines are main Fortran/C issues
- Originally derived from needs of LINPACK / EISPACK then LAPACK
- Four precisions: single, double, single complex, double complex
  - "s", "d", "c", "z" prefixes
- Level-1: Vector-vector operations
  - Double precision vector addition = "daxpy"
- Level-2: Matrix-vector operations
  - Double precision matrix-vector product = "dgemv"
- Level-3: Matrix-matrix operations
  - Double precision matrix-matrix product = "dgemm"
- There are also sparse BLAS and a next-generation BLAS, but neither are well-supported by vendors

# BLAS

- (Updated set of) Basic Linear Algebra Subprograms

- The BLAS functionality is divided into three levels:
  - **Level 1:** contains vector operations of the form:

    $$\mathbf{y} \leftarrow \alpha\mathbf{x} + \mathbf{y}$$

    as well as scalar dot products and vector norms

  - **Level 2:** contains matrix-vector operations of the form

    $$\mathbf{y} \leftarrow \alpha A\mathbf{x} + \beta\mathbf{y}$$

    as well as Tx = y solving for x with T being triangular

  - **Level 3:** contains matrix-matrix operations of the form

    $$C \leftarrow \alpha AB + \beta C$$

    as well as solving $B \leftarrow \alpha T^{-1} B$ for triangular matrices T. This level contains the widely used General Matrix Multiply operation.

# BLAS

- Several implementations for different languages exist
  - Reference implementation (F77 and C-wrapper)
    http://www.netlib.org/blas/
  - ATLAS, highly optimized for particular processor architectures
  - A generic C++ template class library providing BLAS functionality: uBLAS
    http://www.boost.org
  - Several vendors provide libraries optimized for their architecture (AMD, HP, IBM, Intel, NEC, NViDIA, Sun)

# BLAS: F77 naming conventions

- Each routine has a name which specifies the operation, the type of matrices involved and their precisions.
  Names are in the form: PMMOO
  - Some of the most common operations (OO):
    - **DOT** scalar product, x^T y
      **AXPY** vector sum, α x + y
      **MV** matrix-vector product, A x
      **SV** matrix-vector solve, inv(A) x
      **MM** matrix-matrix product, A B
      **SM** matrix-matrix solve, inv(A) B
  - The types of matrices are (MM)
    - **GE** general
      **GB** general band
      **SY** symmetric
      **SB** symmetric band
      **SP** symmetric packed
      **HE** hermitian
      **HB** hermitian band
      **HP** hermitian packed
      **TR** triangular
      **TB** triangular band
      **TP** triangular packed
  - Each operation is defined for four precisions (P)
    - **S** single real
      **D** double real
      **C** single complex
      **Z** double complex
- Examples

  **SGEMM** stands for “single-precision general matrix-matrix multiply”

  **DGEMM** stands for “double-precision matrix-matrix multiply”.

# BLAS: C naming conventions

- F77 routine name is changed to lowercase and prefixed with cblas_
- All routines accepting two dimensional arrays have a new additional first parameter specifying the matrix memory layout (row major or column major)
- Character parameters are replaced by corresponding enum values
- Input arguments are declared const
- Non-complex scalar input parameters are passed by value
- Complex scalar input arguments are passed using a void*
- Arrays are passed by address
- Output scalar arguments are passed by address
- Complex functions become subroutines which return the result via an additional last parameter (void*), appending _sub to the name

# _axpy

## cblas_daxpy

Computes a constant times a vector plus a vector (double-precision).

```
void cblas_daxpy (
   const int N,
   const double alpha,
   const double *X,
   const int incX,
   double *Y,
   const int incY
);
```

**Parameters**

*N*
Number of elements in the vectors.

*alpha*
Scaling factor for the values in `X`.

*X*
Input vector `X`.

*incX*
Stride within `X`. For example, if `incX` is 7, every 7th element is used.

*Y*
Input vector `Y`.

*incY*
Stride within `Y`. For example, if `incY` is 7, every 7th element is used.

**Discussion**

On return, the contents of vector Y are replaced with the result. The value computed is `(alpha * X[i]) + Y[i]`.

**Availability**

Available in OS X v10.2 and later.

**Declared In**

`cblas.h`

# cblas_dgemm

## cblas_dgemm

Multiplies two matrices (double-precision).

```
void cblas_dgemm (
    const enum CBLAS_ORDER Order,
    const enum CBLAS_TRANSPOSE TransA,
    const enum CBLAS_TRANSPOSE TransB,
    const int M,
    const int N,
    const int K,
    const double alpha,
    const double *A,
    const int lda,
    const double *B,
    const int ldb,
    const double beta,
    double *C,
    const int ldc
);
```

**Parameters**

*Order*
Specifies row-major (C) or column-major (Fortran) data ordering.

*TransA*
Specifies whether to transpose matrix `A`.

*TransB*
Specifies whether to transpose matrix `B`.

*M*
Number of rows in matrices `A` and `C`.

*N*
Number of columns in matrices `B` and `C`.

*K*
Number of columns in matrix `A`; number of rows in matrix `B`.

*alpha*
Scaling factor for the product of matrices A and B.

*A*
Matrix A.

*lda*
The size of the first dimention of matrix `A`; if you are passing a matrix `A[m][n]`, the value should be `m`.

*B*
Matrix B.

*ldb*
The size of the first dimention of matrix `B`; if you are passing a matrix `B[m][n]`, the value should be `m`.

*beta*
Scaling factor for matrix C.

*C*
Matrix C.

*ldc*
The size of the first dimention of matrix `C`; if you are passing a matrix `C[m][n]`, the value should be `m`.

# Basic Linear Algebra Subprograms (BLAS)

- Level 1: Vector-Vector operations

| name | description | equation | prefixes |
|---|---|---|---|
| _rotg | generate plane rotation | | s, d |
| _rotmg | generate modified plane rotation | | s, d |
| _rot | apply plane rotation | | s, d |
| _rotm | apply modified plane rotation | | s, d |
| _swap | swap vectors | $x \leftrightarrow y$ | s, d, c, z |
| _scal | scale vector | $y = \alpha y$ | s, d, c, z, cs, zd |
| _copy | copy vector | $y = x$ | s, d, c, z |
| _axpy | update vector | $y = y + \alpha x$ | s, d, c, z |
| _dot | dot product | $= x^t y$ | s, d, ds |
| _dotc | complex conj dot | $= x^h y$ | c, z |
| _dotu | complex dot | $= x^t y$ | c, z |
| __dot | | $= \alpha + x^t y$ | sds |
| _nrm2 | 2-norm | $= \|x\|_2$ | s, d, sc, dz |
| _asum | 1-norm | $= \|\mathrm{Re}(x)\|_1 + \|\mathrm{Im}(x)\|_1$ | s, d, sc, dz |
| i_amax | ∞-norm | $= i$ such that $\lvert\mathrm{Re}(x_i)\rvert + \lvert\mathrm{Im}(x_i)\rvert$ is max | s, d, c, z |

| name | description | equation | prefixes |
|---|---|---|---|
| _gemv | general matrix-vector multiply | $y = \alpha A^* x + \beta y$ | s, d, c, z |
| _gbmv | (banded) | $y = \alpha A^* x + \beta y$ | s, d, c, z |
| _hemv | hermetian mat-vec | $y = \alpha A x + \beta y$ | c, z |
| _hbmv | (banded) | $y = \alpha A x + \beta y$ | c, z |
| _hpmv | (packed) | $y = \alpha A x + \beta y$ | c, z |
| _symv | symmetric mat-vec | $y = \alpha A x + \beta y$ | s, d, (c, z)† |
| _sbmv | (banded) | $y = \alpha A x + \beta y$ | s, d |
| _spmv | (packed) | $y = \alpha A x + \beta y$ | s, d, (c, z)† |
| _trmv | triangular mat-vec | $x = A^* x$ | s, d, c, z |
| _tbmv | (banded) | $x = A^* x$ | s, d, c, z |
| _tpmv | (packed) | $x = A^* x$ | s, d, c, z |
| _trsv | triangular solve | $x = A^{-*} x$ | s, d, c, z |
| _tbsv | (banded) | $x = A^{-*} x$ | s, d, c, z |
| _tpsv | (packed) | $x = A^{-*} x$ | s, d, c, z |

$A^*$ denotes $A$, $A^T$, or $A^H$;
$A^{-*}$ denotes $A^{-1}$, $A^{-T}$, or $A^{-H}$, depending on options and data type.
$A$ is $m \times n$ or $n \times n$

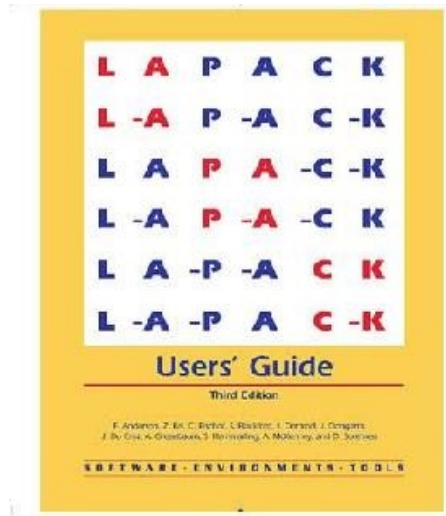
| name | description | equation | prefixes |
|---|---|---|---|
| _ger | general rank-1 update | $A = A + \alpha x y^T$ | s, d |
| _geru | (complex) | $A = A + \alpha x y^T$ | c, z |
| _gerc | (complex conj) | $A = A + \alpha x y^H$ | c, z |
| _her | hermetian rank-1 update | $A = A + \alpha x x^H$ | c, z |
| _hpr | (packed) | $A = A + \alpha x x^H$ | c, z |
| _her2 | hermetian rank-2 update | $A = A + \alpha x y^H + y(\alpha x)^H$ | c, z |
| _hpr2 | (packed) | $A = A + \alpha x y^H + y(\alpha x)^H$ | c, z |
| _syr | symmetric rank-1 update | $A = A + \alpha x x^T$ | s, d, (c, z)† |
| _spr | (packed) | $A = A + \alpha x x^T$ | s, d, (c, z)† |
| _syr2 | symmetric rank-2 update | $A = A + \alpha x y^T + \alpha y x^T$ | s, d |
| _spr2 | (packed) | $A = A + \alpha x y^T + \alpha y x^T$ | s, d |

| name | description | equation | prefixes |
|---|---|---|---|
| _gemm | general matrix-matrix multiply | $C = \alpha A^* B^* + \beta C$ | s, d, c, z |
| _symm | symmetric mat-mat | $C = \alpha AB + \beta C$ | s, d, c, z |
| _hemm | hermetian mat-mat | $C = \alpha AB + \beta C$ | c, z |
| _syrk | symmetric rank-$k$ update | $C = \alpha AA^T + \beta C$ | s, d, c, z |
| _herk | hermetian rank-$k$ update | $C = \alpha AA^H + \beta C$ | c, z |
| _syr2k | symmetric rank-2$k$ update | $C = \alpha AB^T + \bar{\alpha} BA^T + \beta C$ | s, d, c, z |
| _her2k | hermetian rank-2$k$ update | $C = \alpha AB^H + \bar{\alpha} BA^H + \beta C$ | c, z |
| _trmm | triangular mat-mat | $B = \alpha A^* B$ or $B = \alpha BA^*$ | s, d, c, z |
| _trsm | triangular solve mat | $B = \alpha A^{-*} B$ or $B = \alpha BA^{-*}$ | s, d, c, z |

$A^*$ denotes $A$, $A^T$, or $A^H$;
$A^{-*}$ denotes $A^{-1}$, $A^{-T}$, or $A^{-H}$, depending on options and data type.
The destination matrix is $m \times n$ or $n \times n$. For mat-mat, the common dimension of $A$ and $B$ is $k$.

# LAPACK

- F77, based on blocked algorithms (BLAS 3)
- Driver routines (simple and expert) used to solve a complete problem
  - Solve a linear system of equations
  - Least squares solutions
  - Eigenvalue problems
  - Singular value problems
- Routines for distinct computational tasks
  - LU / Cholesky / QR / SVD factorization
  - Schur / generalized Schur decomposition
- Auxiliary
  - Estimate condition numbers
  - Unblocked algorithms
  - Future extensions to BLAS




http://www.netlib.org/lapack

# LAPACK naming conventions

- Similar to BLAS
  - **XYYZZZ**
    - **X**: data type
      - **S**: REAL
      - **D**: DOUBLE PRECISION
      - **C**: COMPLEX
      - **Z**: COMPLEX*16 or DOUBLE COMPLEX
    - **YY**: matrix type
      - **BD**: bidiagonal
      - **DI**: diagonal
      - **GB**: general band
      - **GE**: general (i.e., unsymmetric, in some cases rectangular)
      - **GG**: general matrices, generalized problem (i.e., a pair of general matrices)
      - **GT**: general tridiagonal
      - **HB**: (complex) Hermitian band
      - **HE**: (complex) Hermitian
      - **HG**: upper Hessenberg matrix, generalized problem (i.e a Hessenberg and a triangular matrix)
      - **HP**: (complex) Hermitian, packed storage
      - **HS**: upper Hessenberg
      - **OP**: (real) orthogonal, packed storage
      - **OR**: (real) orthogonal
      - **PB**: symmetric or Hermitian positive definite band

- **YY**: more matrix types
  - **PO**: symmetric or Hermitian positive definite
  - **PP**: symmetric or Hermitian positive definite, packed storage
  - **PT**: symmetric or Hermitian positive definite tridiagonal
  - **SB**: (real) symmetric band
  - **SP**: symmetric, packed storage
  - **ST**: (real) symmetric tridiagonal
  - **SY**: symmetric
  - **TB**: triangular band
  - **TG**: triangular matrices, generalized problem (i.e., a pair of triangular matrices)
  - **TP**: triangular, packed storage
  - **TR**: triangular (or in some cases quasi-triangular)
  - **TZ**: trapezoidal
  - **UN**: (complex) unitary
  - **UP**: (complex) unitary, packed storage
- **ZZZ**: performed computation
  - Linear systems
  - Factorizations
  - Eigenvalue problems
  - Singular value decomposition
  - Etc.

# Roofline Model

- Performance: locality, locality, locality
- Because computation is really really fast
- And moving data is expensive
- Limits on performance: Bandwidth, Latency, Peak Compute

$$\text{Performance} = \frac{\text{GFlops}}{\text{second}} = \min \begin{cases} \text{CPU Peak} \\ \text{Bandwidth} \end{cases}$$

Williams, Samuel, Andrew Waterman, and David Patterson. "Roofline: an insightful visual performance model for multicore architectures." *Communications of the ACM* 52.4 (2009): 65-76.

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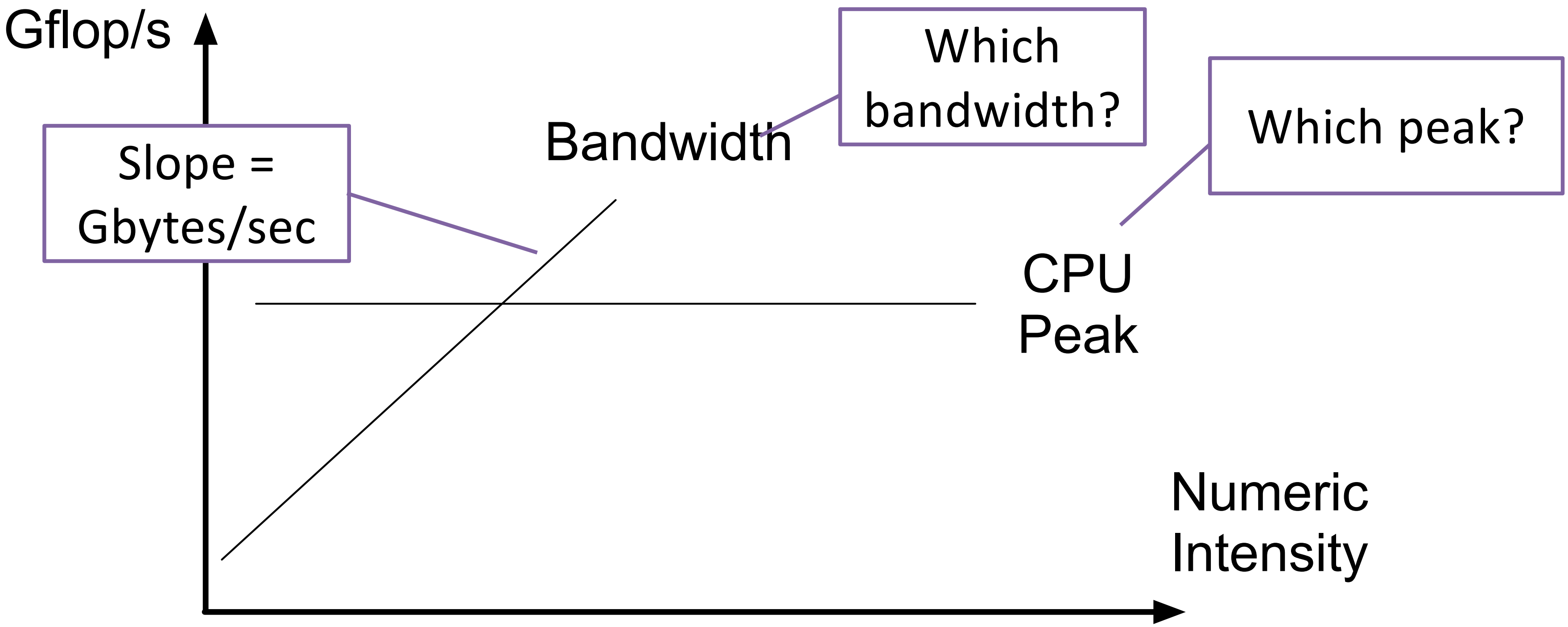
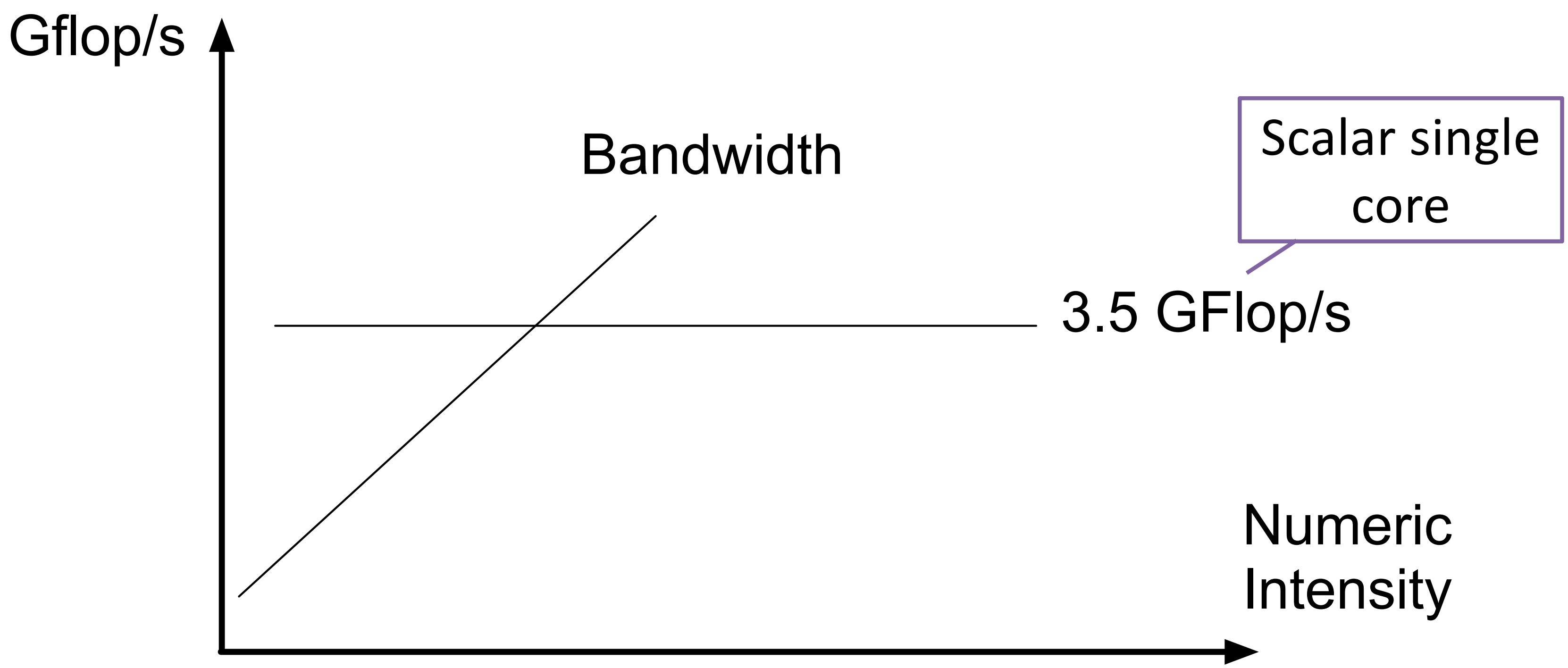
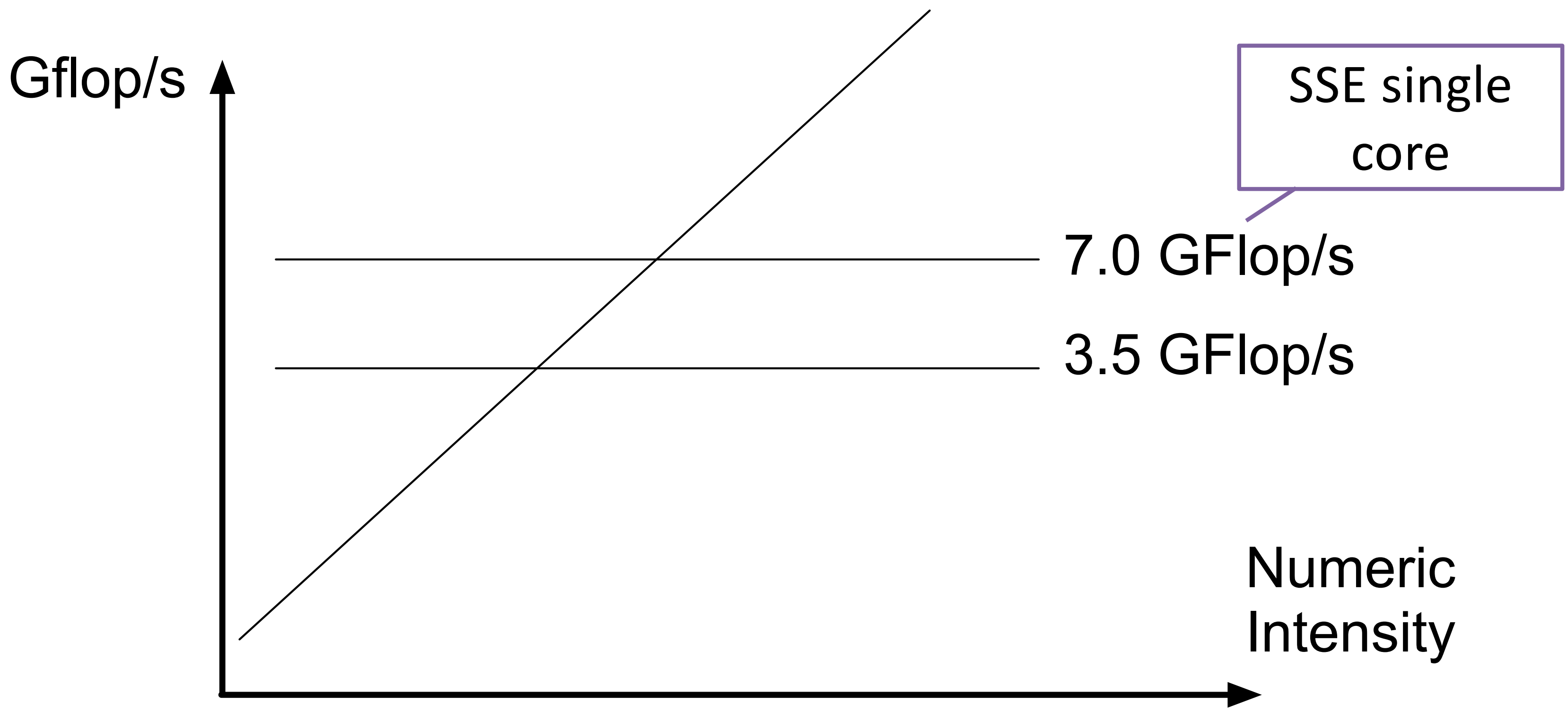


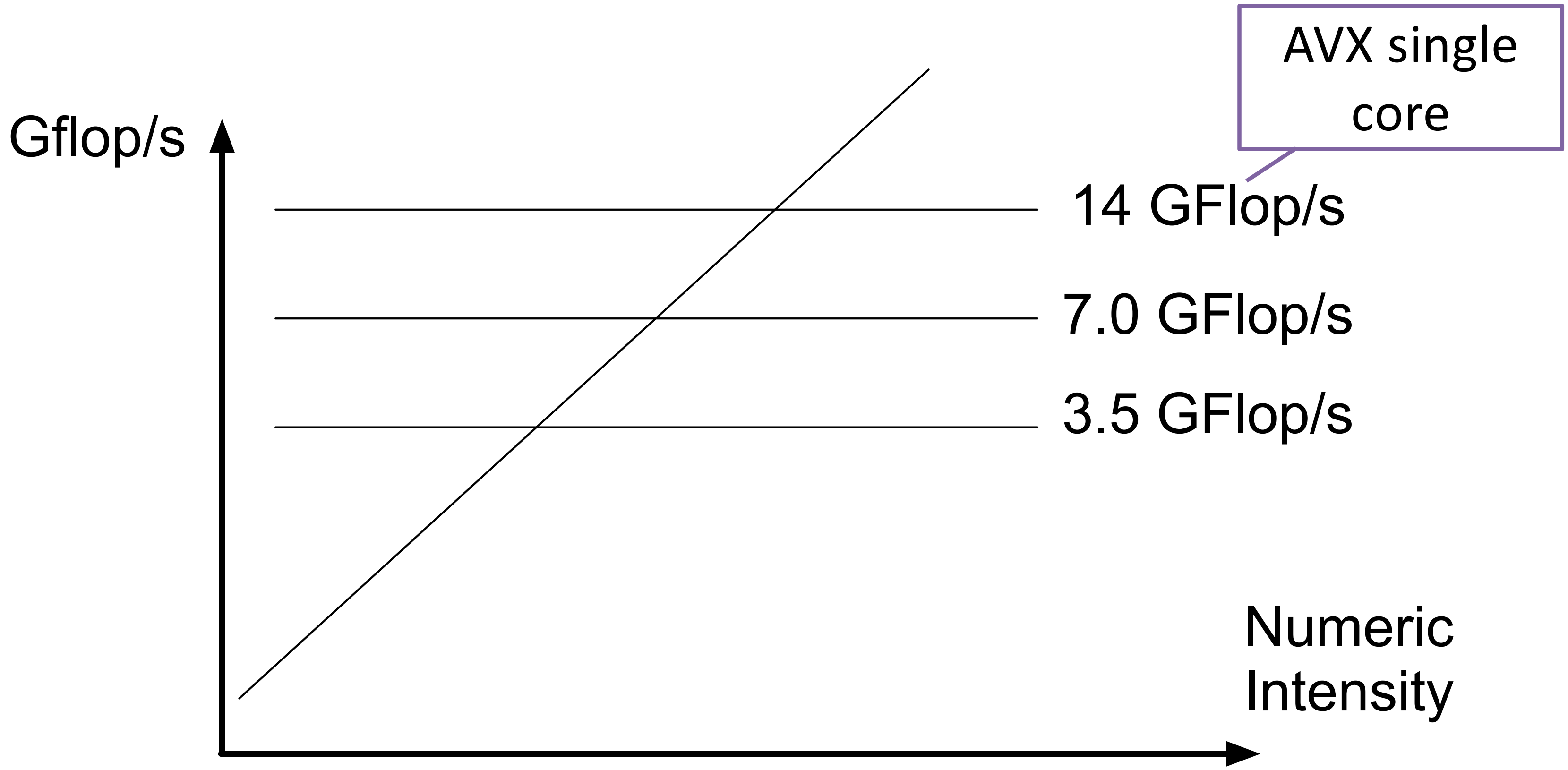
# Roofline Model



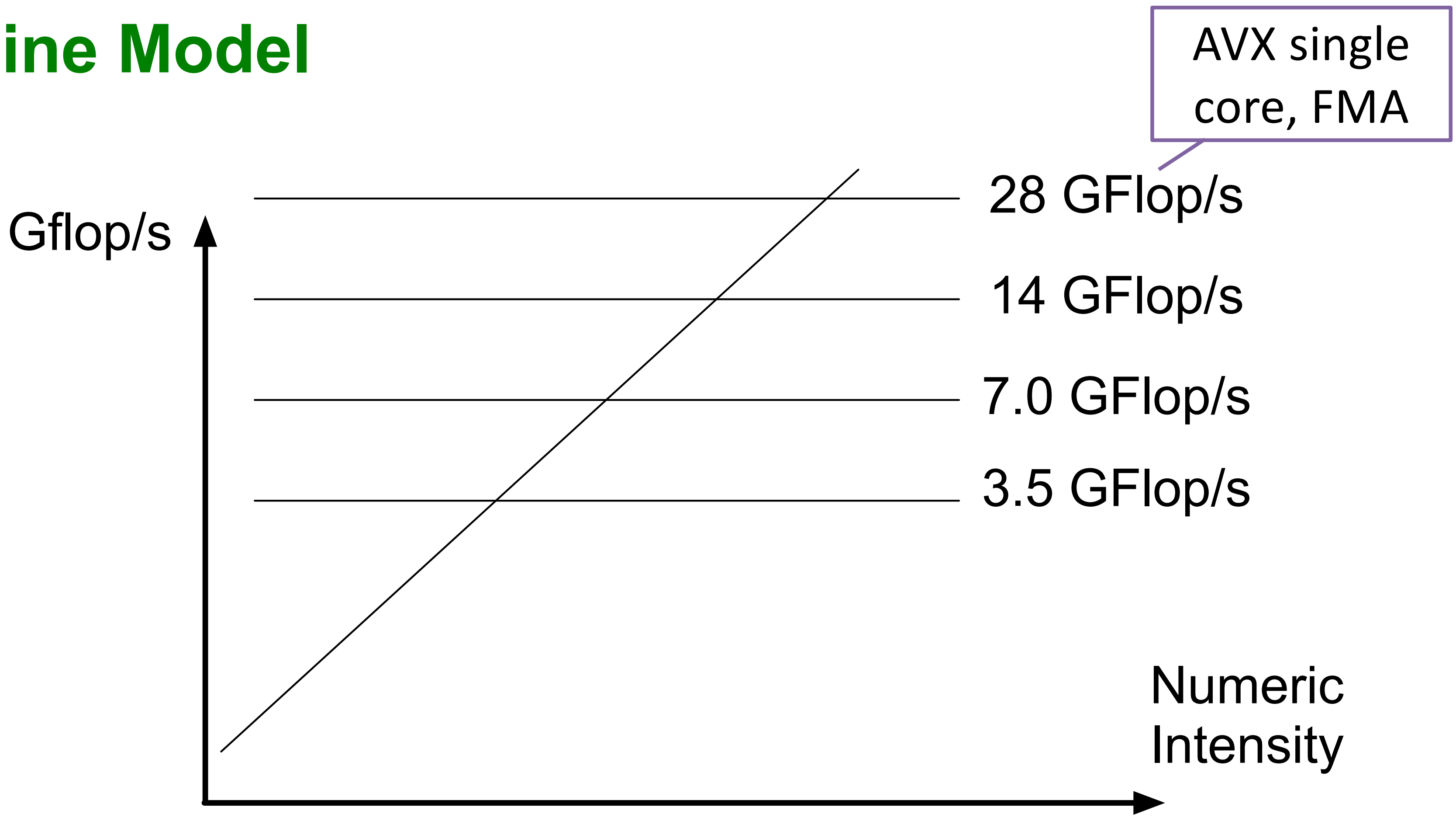
# Roofline Model



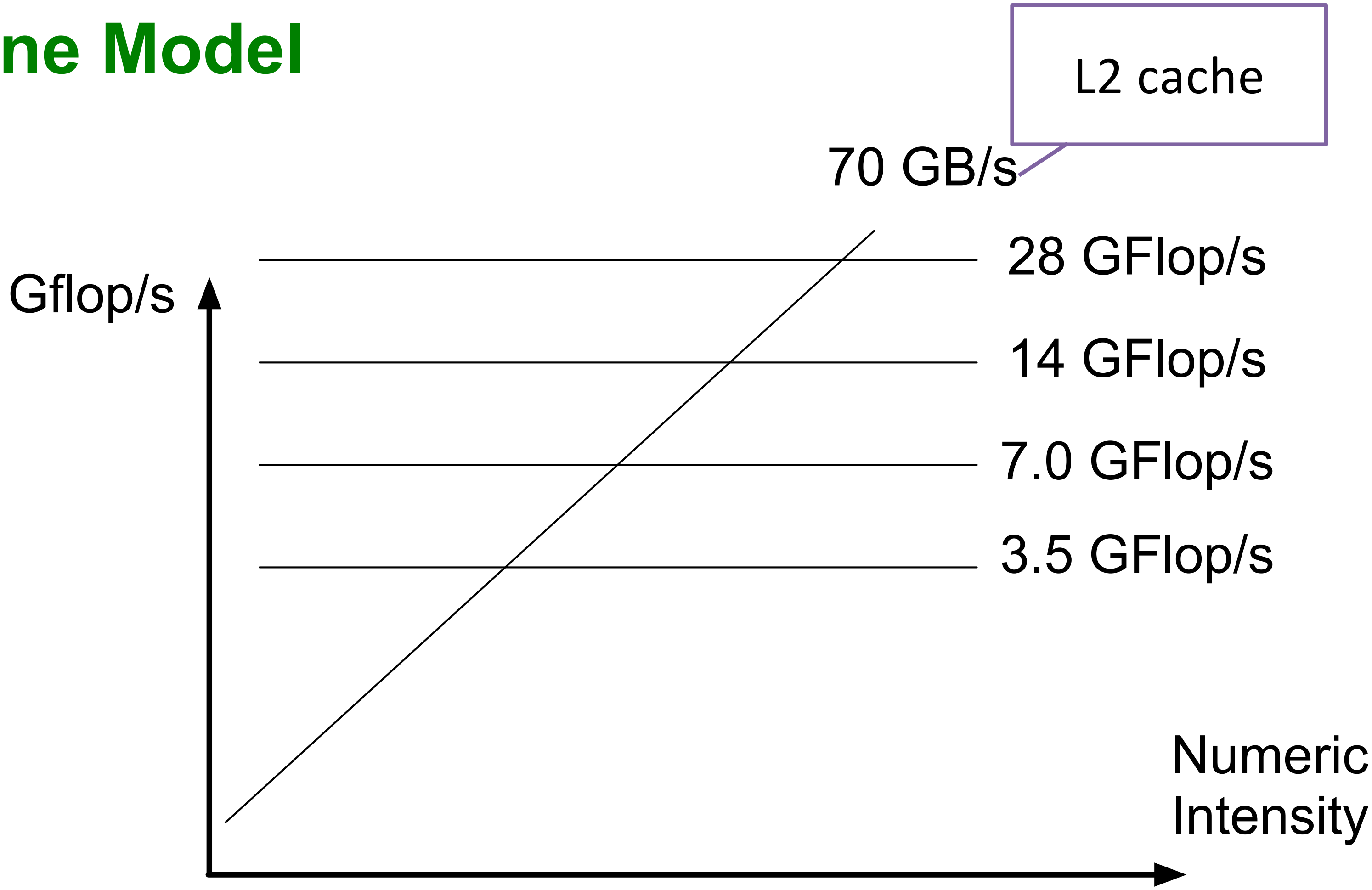
# Roofline Model



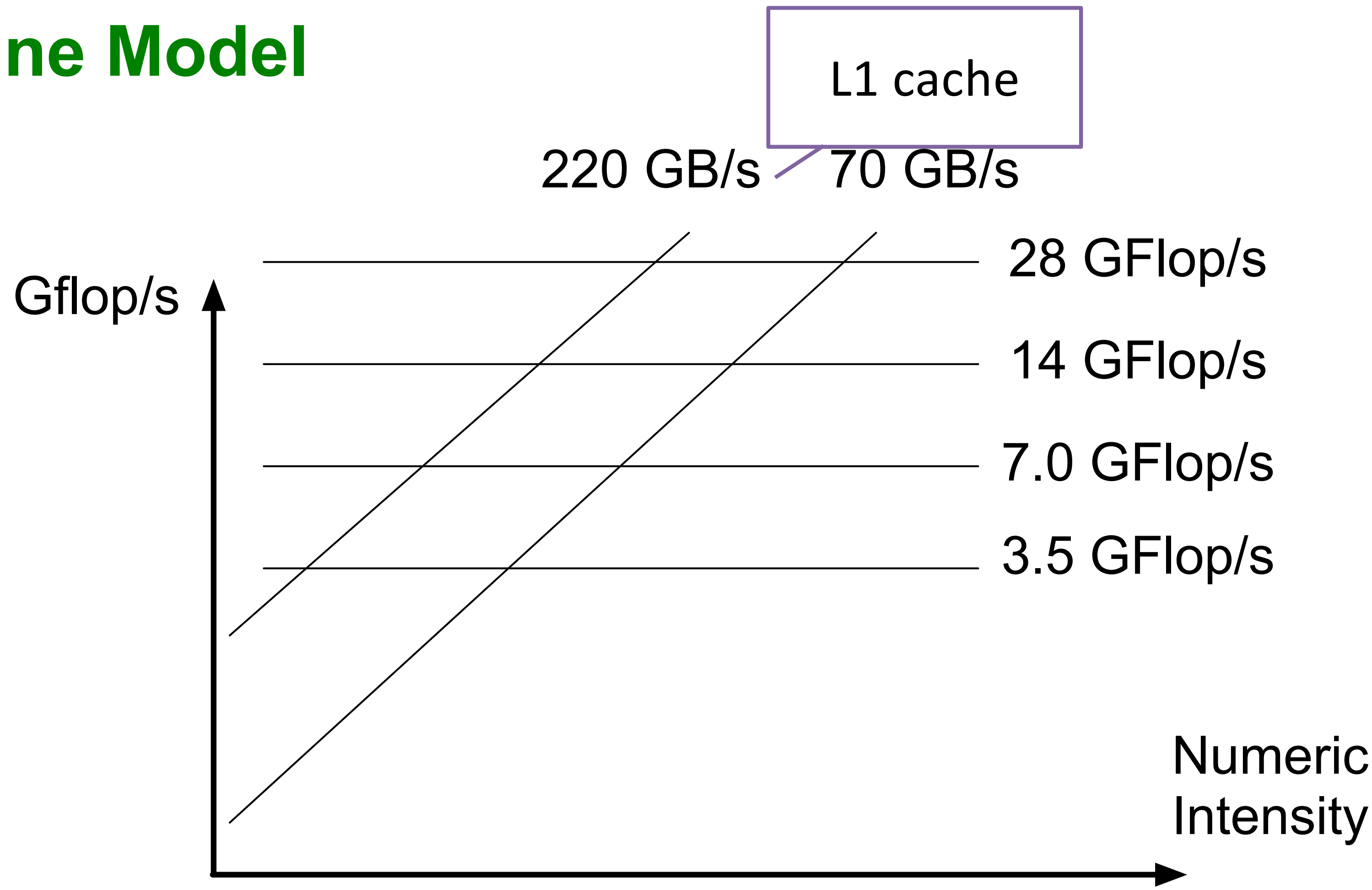
# Roofline Model



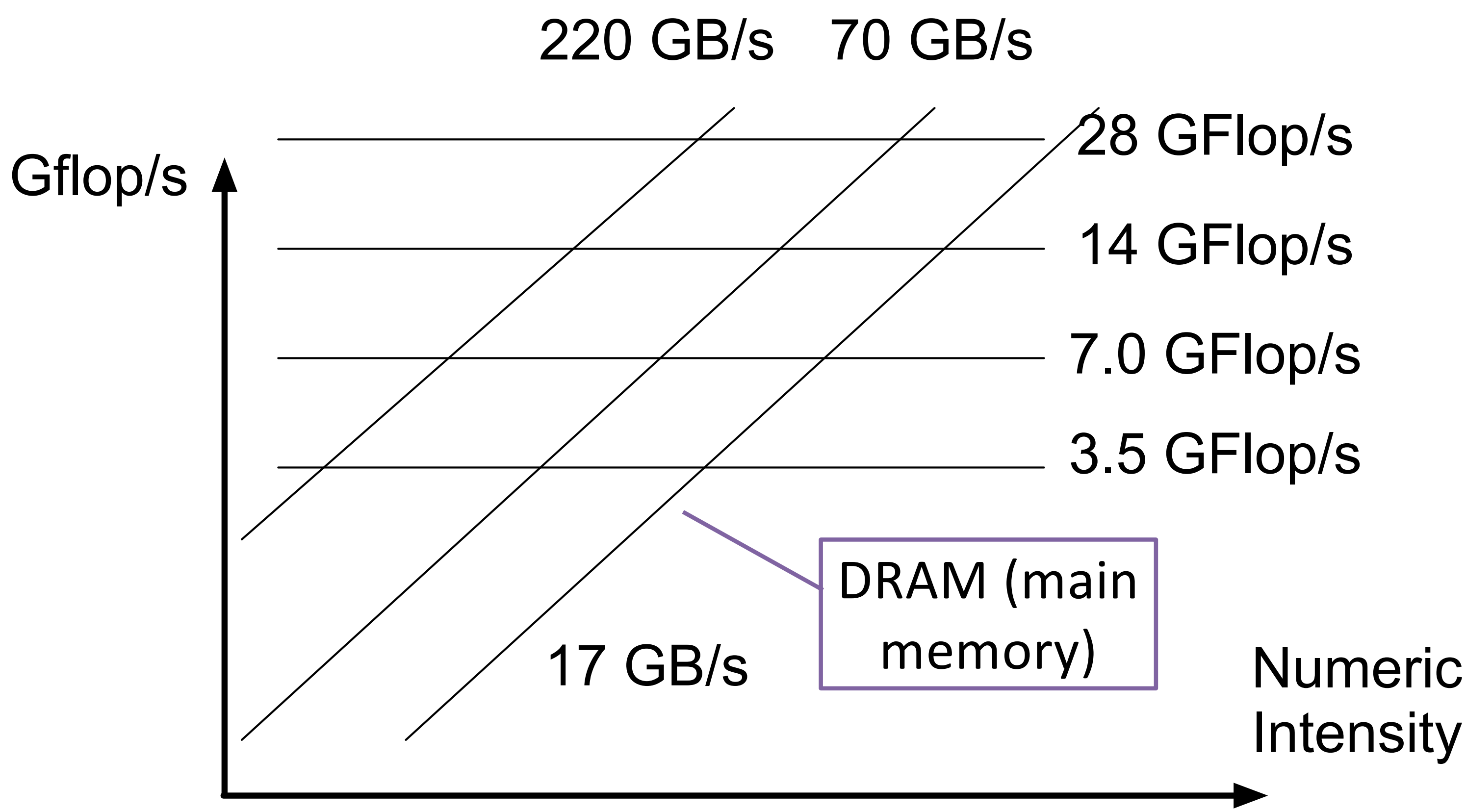
# Roofline Model



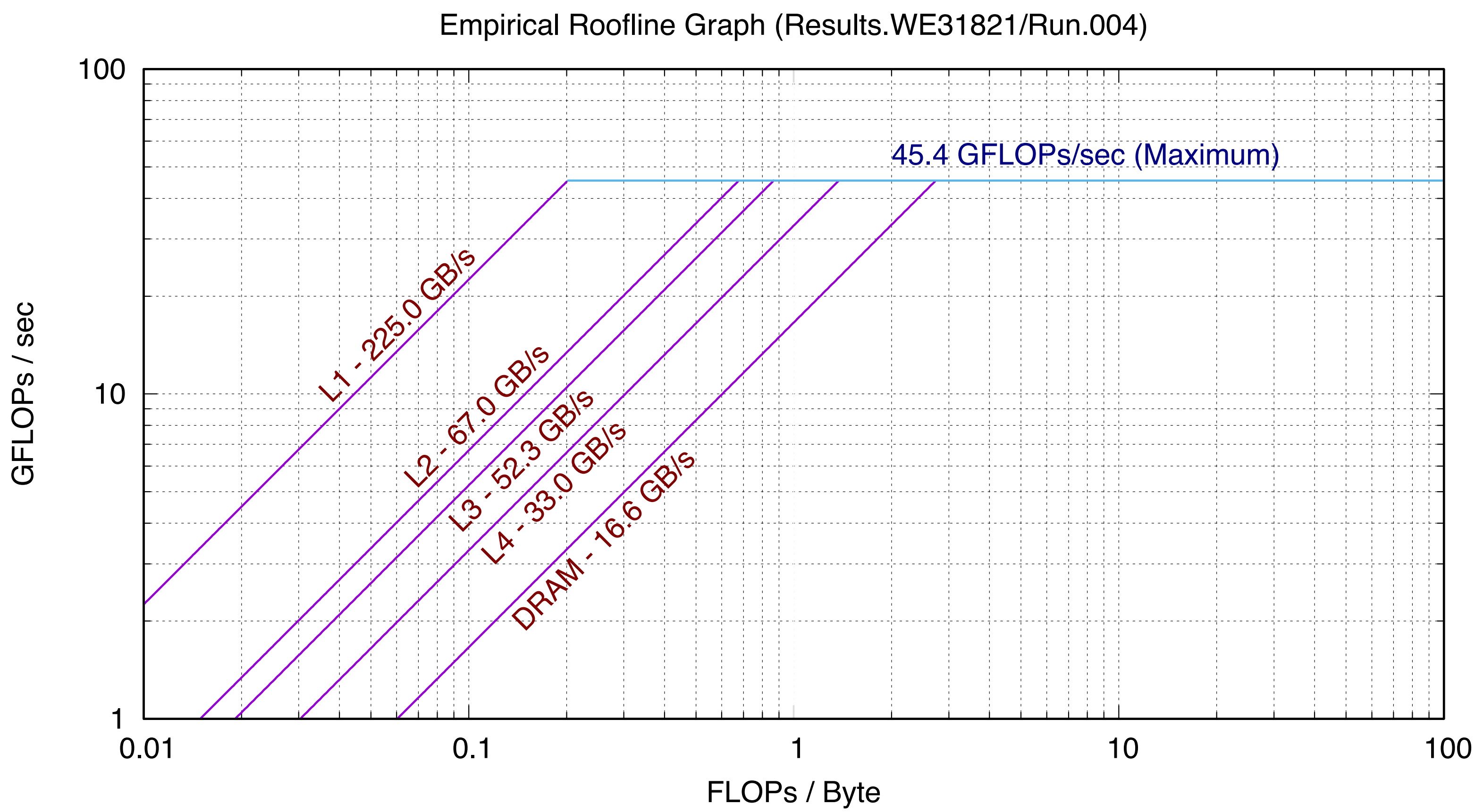
# Roofline Model



# Roofline Model



# Measured


Empirical Roofline Graph (Results.WE31821/Run.004)
45.4 GFLOPs/sec (Maximum)
L1 - 225.0 GB/s
L2 - 67.0 GB/s
L3 - 52.3 GB/s
L4 - 33.0 GB/s
DRAM - 16.6 GB/s
GFLOPs / sec
FLOPs / Byte
100
10
1
0.01
0.1
1
10
100

# Numerical Intensity

```
void matvec_dense(const Matrix& A, const Vector& x, Vector& y) {
  for (size_t i = 0; i < A.num_rows(); ++i) {
    for (size_t j = 0; j < A.num_cols(); ++j) {
      y(i) += A(i, j) * x(j);
    }
  }
}
```

Three doubles = 24 bytes?

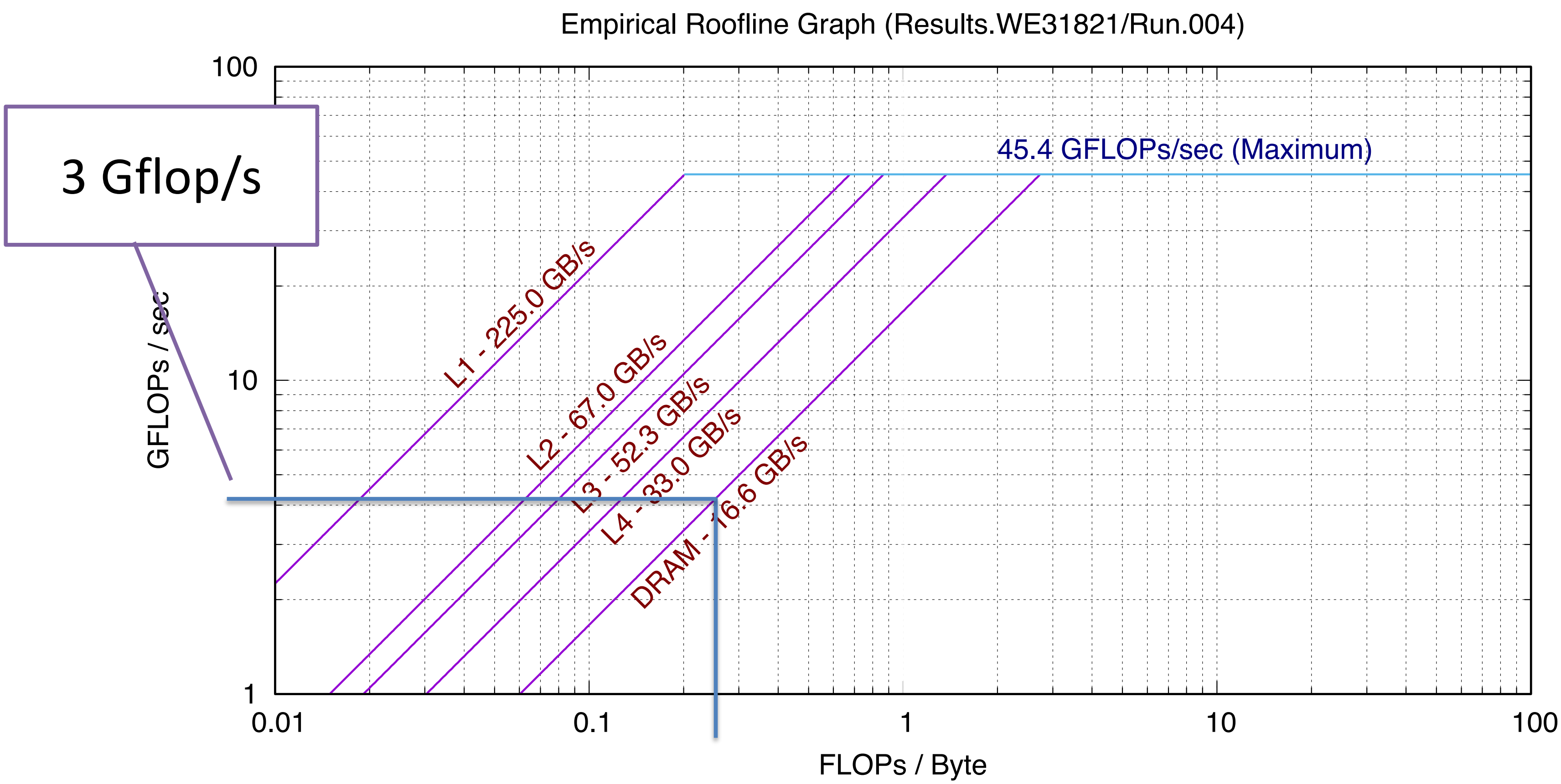
Two flops

$2N^2$ Flops

$(N^2 + 2N)$ doubles $= 8(N^2 + 2N)$ bytes

$\frac{1}{4} \frac{\text{Flop}}{\text{byte}}$

# Measured



Empirical Roofline Graph (Results.WE31821/Run.004)
3 Gflop/s
45.4 GFLOPs/sec (Maximum)
L1 - 225.0 GB/s
L2 - 67.0 GB/s
L3 - 52.3 GB/s
L4 - 33.0 GB/s
DRAM - 16.6 GB/s
GFLOPs / sec
FLOPs / Byte
100
10
1
0.01
0.1
1
10
100

# Numerical Intensity

```
void matvec(const Vector& x, Vector& y) const {
  for (size_type k = 0; k < arrayData.size(); ++k) {
    y(rowIndices[k]) += arrayData[k] * x(rowIndices[k]);
  }
}
```

Three doubles + 2 ints
= 32 bytes? (36 bytes?)

Two flops

2 NNZ Flops

5N

$\text{NNZ doubles}$
$+2\ \text{NNZ indexes}$
$+2N\ \text{doubles}$

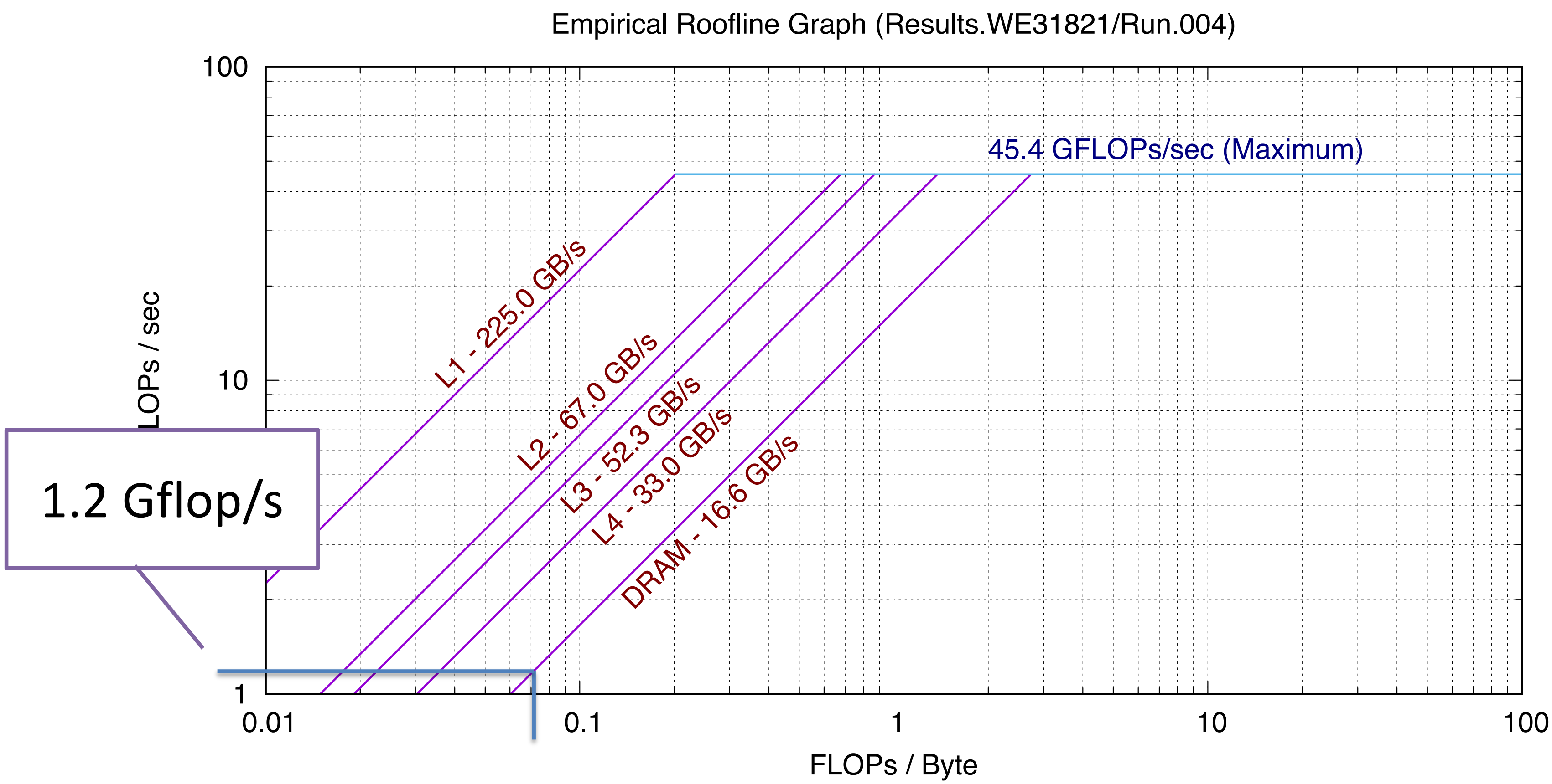
$\frac{1}{14}\ \frac{\text{Flop}}{\text{byte}}$

10N Flops

7N doubles = 56 bytes

10N indexes = 40, 80 bytes

# Measured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100
10
1
0.01
0.1
1
10
100
FLOPs / Byte
LOPs / sec
1.2 Gflop/s

# Numerical Intensity

```
void matmat_dense(const Matrix& A, const Matrix& B, Matrix& C) {
  for (size_t i = 0; i < C.num_rows(); ++i) {
    for (size_t j = 0; j < C.num_cols(); ++j) {
      for (size_t k = 0; k < A.num_cols(); ++k) {
        C(i, j) += A(i, k) * B(k, j);
      }
    }
  }
}
```

Three doubles = 24 bytes?

Two flops

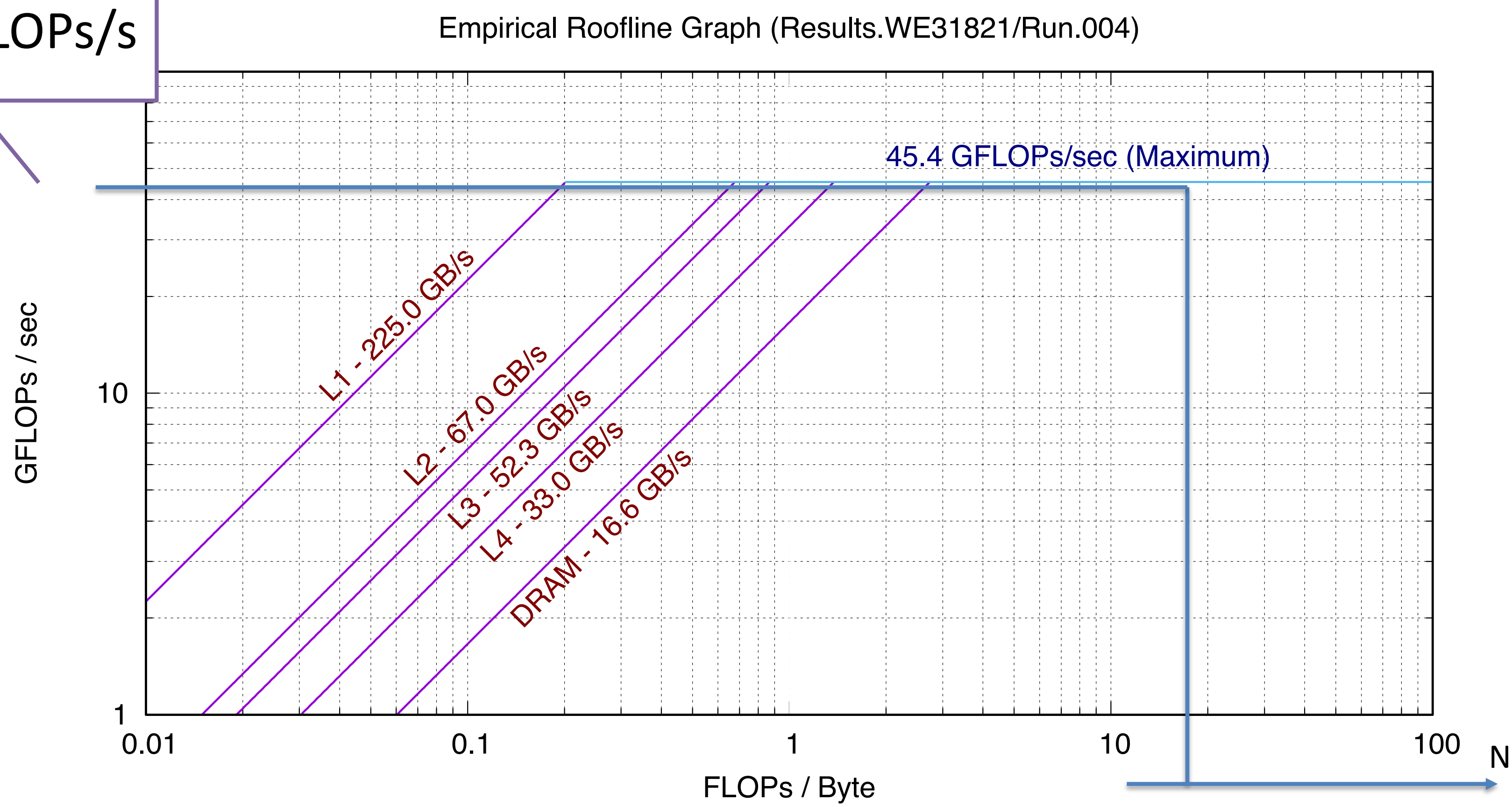
$\frac{N}{12} \frac{\text{Flop}}{\text{byte}}$

$2N^3$ Flops

$3N^2$ doubles $= 24N^2$ bytes

# Measured

45 GFLOPs/s



# Numerical Intensity

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void matmat_dense(const Matrix& A, const Matrix& B, Matrix& C) {
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    }
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}
```

Three doubles = 24 bytes?

Two flops

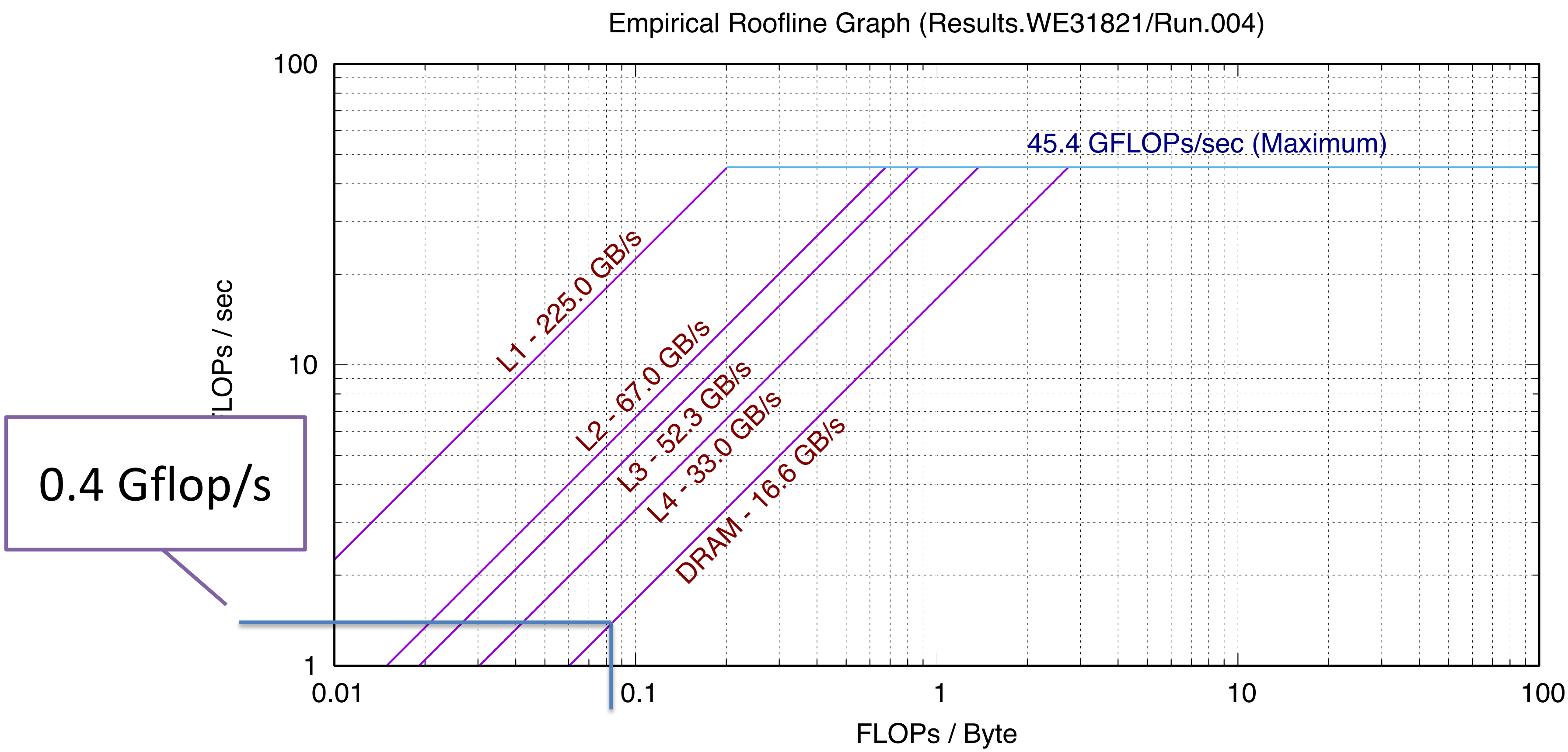
$\frac{1}{12}\frac{\text{Flop}}{\text{byte}}$

$2N^3$ Flops

$3N^3$ doubles $= 24N^3$ bytes

No reuse

# Measured



Empirical Roofline Graph (Results.WE31821/Run.004)
45.4 GFLOPs/sec (Maximum)
L1 - 225.0 GB/s
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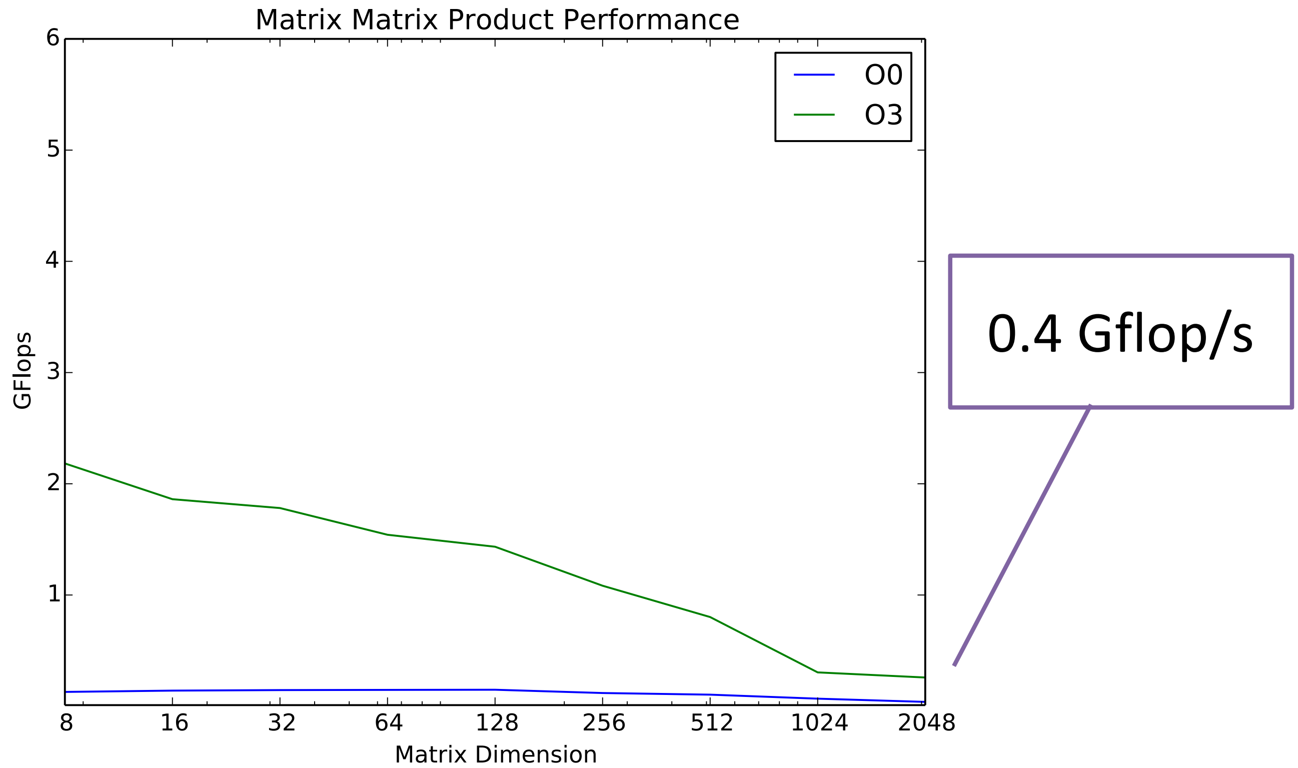
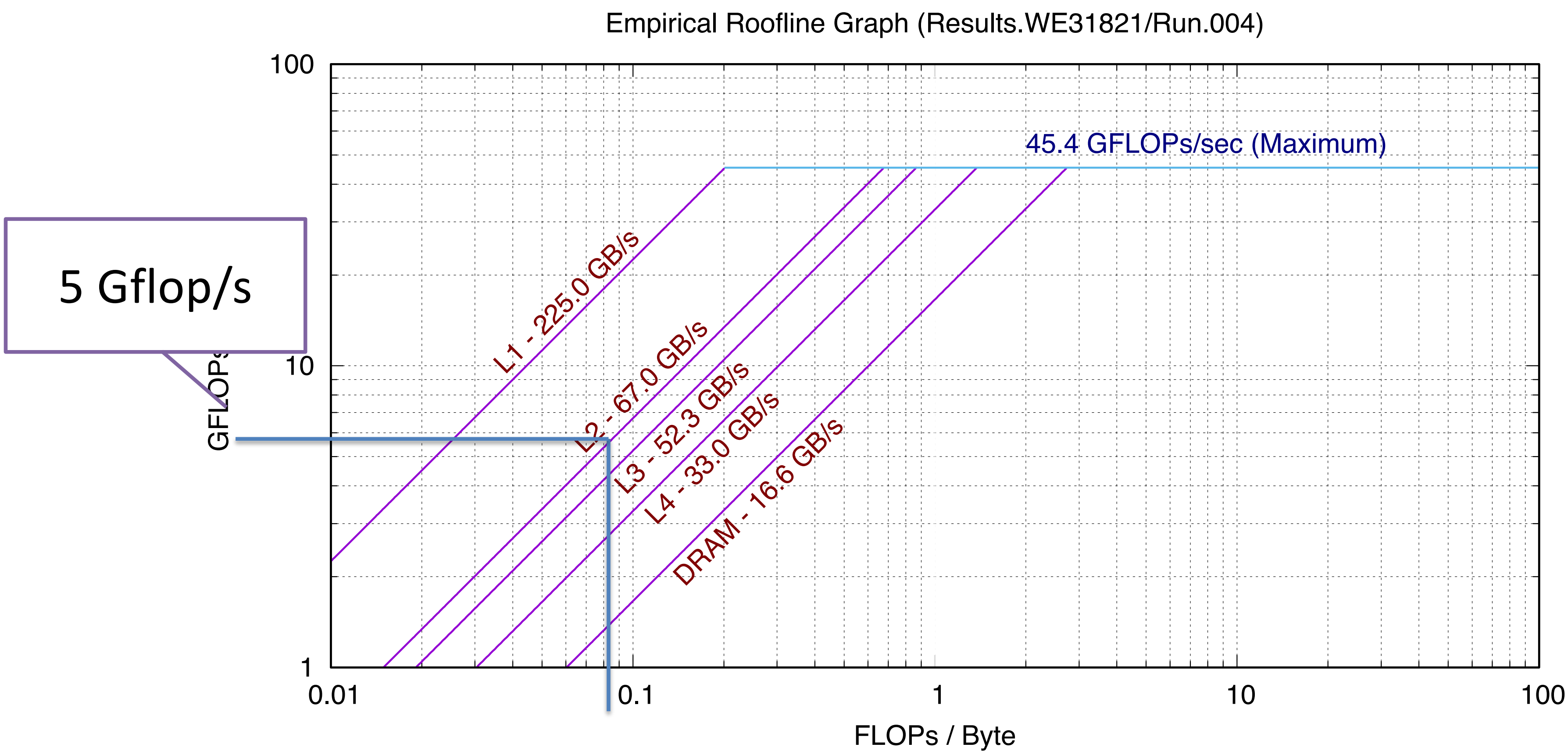
DRAM - 16.6 GB/s
100
10
1
0.01
0.1
1
10
100
FLOPs / Byte
0.4 Gflop/s

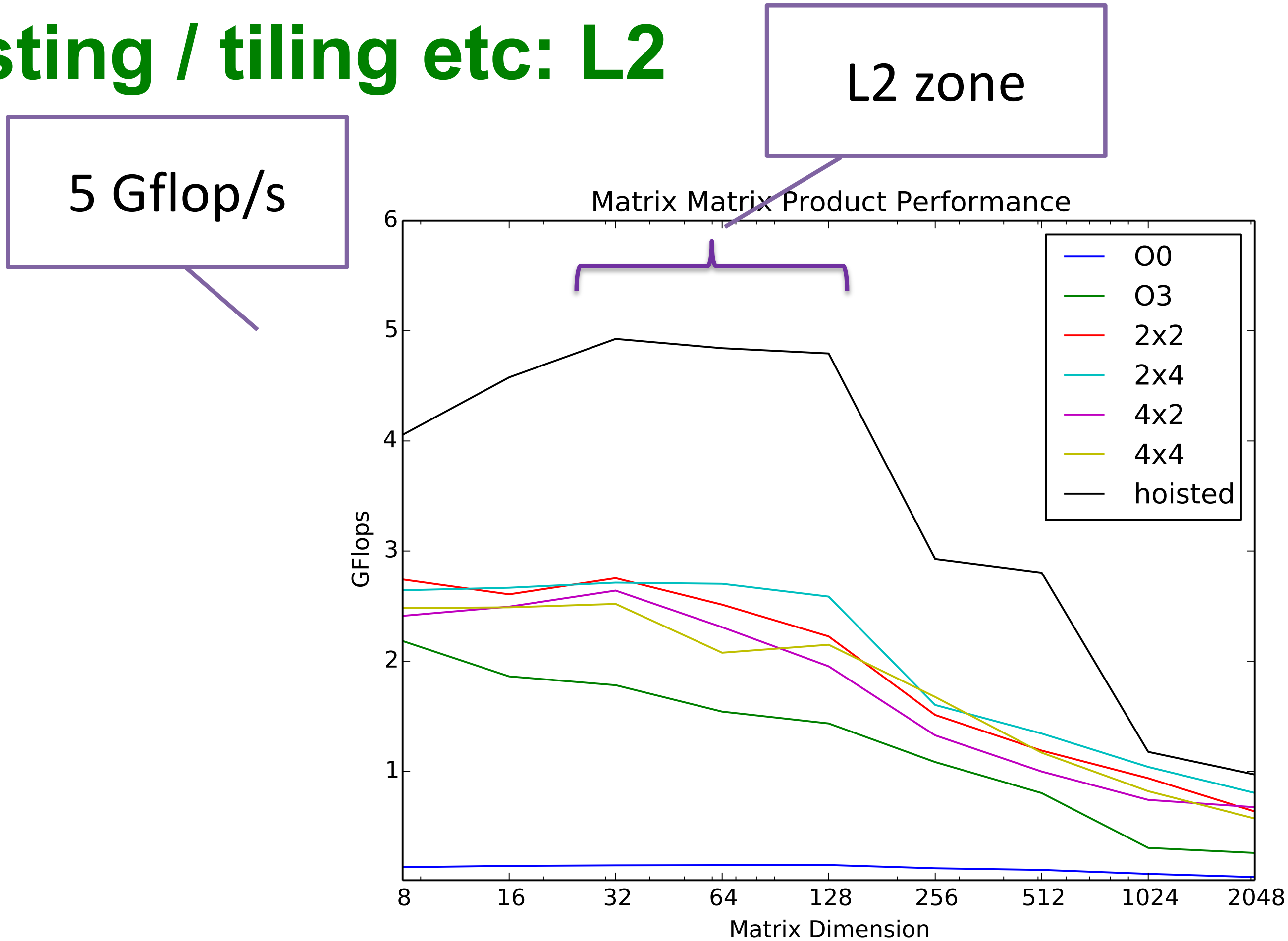
# Recall


Matrix Matrix Product Performance
O0
O3
GFlops
Matrix Dimension
6
5
4
3
2
1
8
16
32
64
128
256
512
1024
2048
0.4 Gflop/s

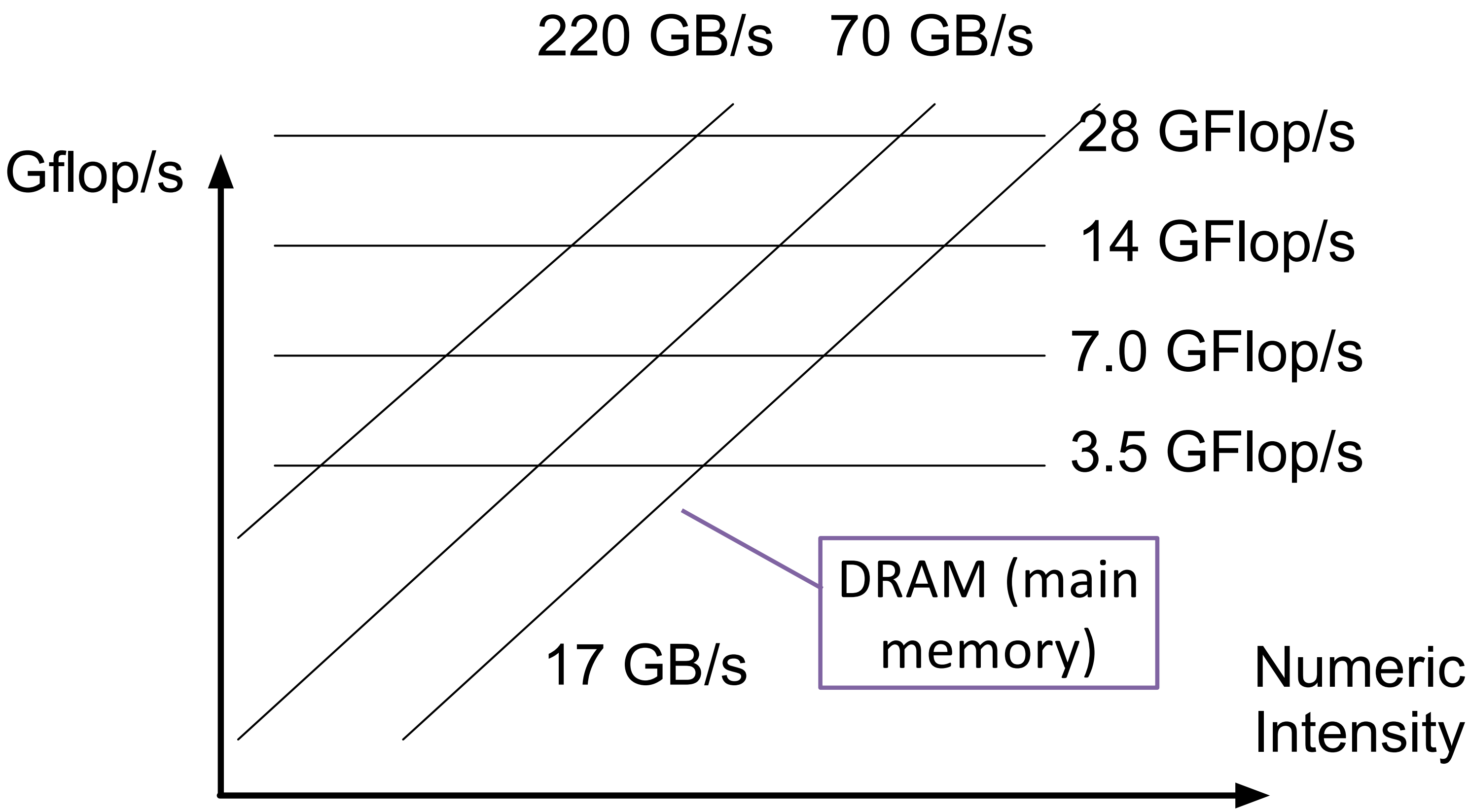
# Hoisting / tiling etc: L2



# Hoisting / tiling etc: L2



# Summary (Roofline Model)



# Thank You!

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