NORTHWEST INSTITUTE for ADVANCED COMPUTING

Pacific Northwest NATIONAL LABORATORY
Proudly Operated by Battelle for the U.S. Department of Energy

UNIVERSITY of WASHINGTON

AMATH 483/583
High Performance Scientific Computing

Lecture 7:
Compilation, optimization, SIMD/Vector

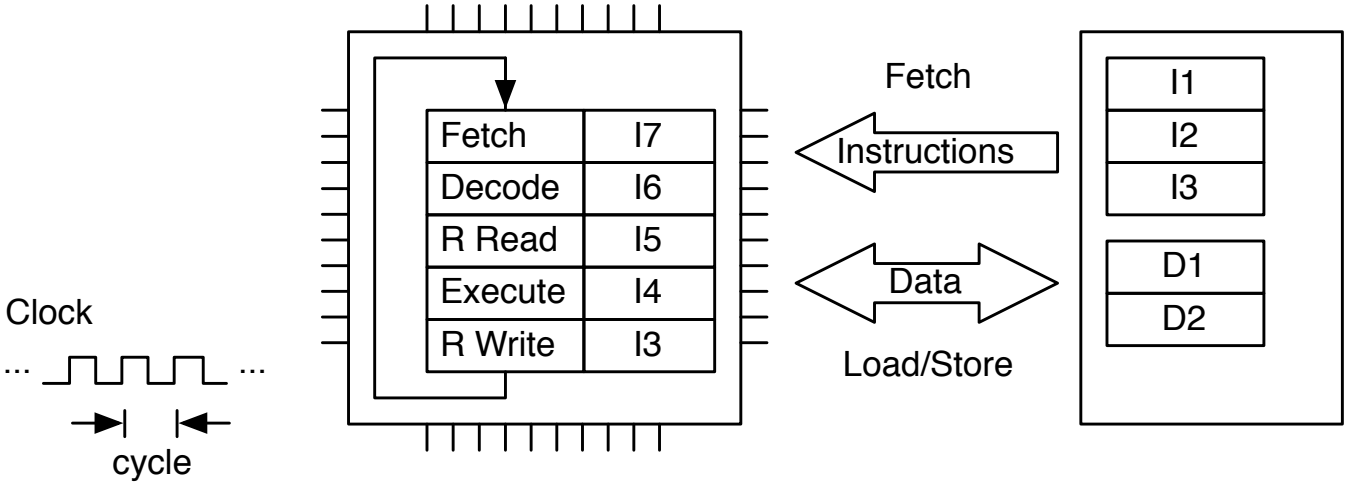
Andrew Lumsdaine
Northwest Institute for Advanced Computing
Pacific Northwest National Laboratory
University of Washington
Seattle, WA

Overview

- Brief review of optimization techniques
- Doing more at once
- Vector instruction sets and intrinsics
- Sparsity

Processor Core Instruction Handling

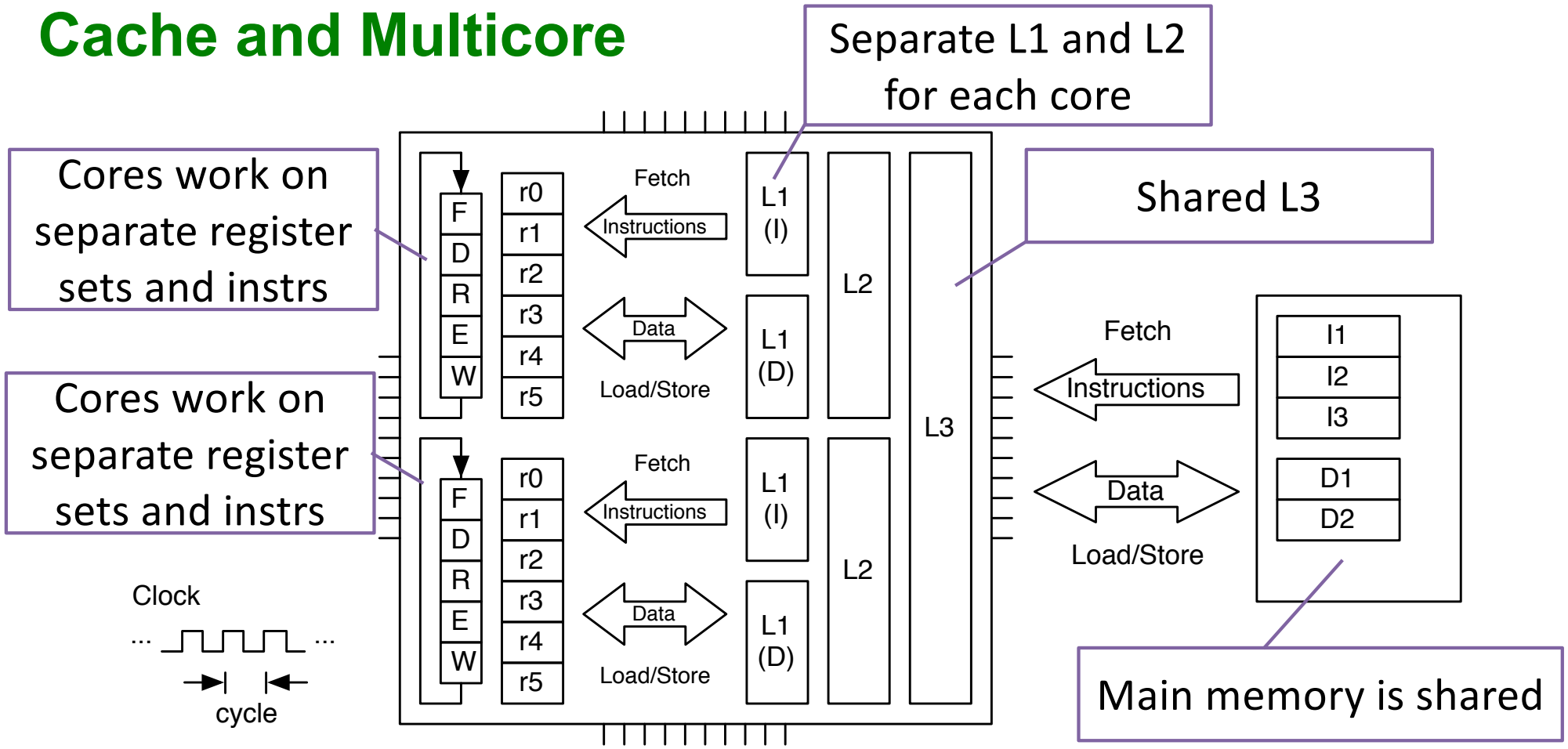
- By pipelining, multiple instructions can be executed at each clock cycle
- Form of instruction-level parallelism (ILP)



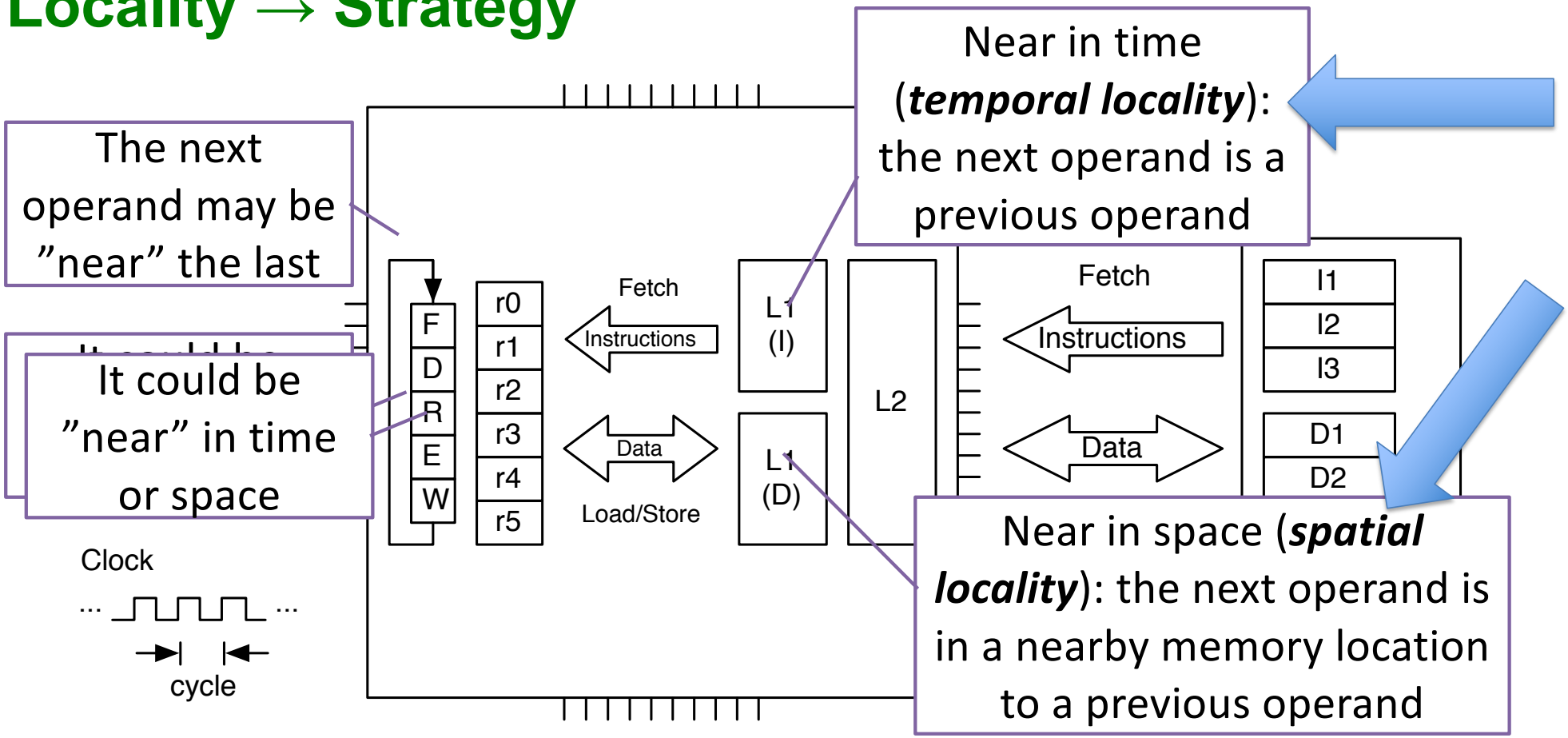
Performance-Oriented Architecture Features

- 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

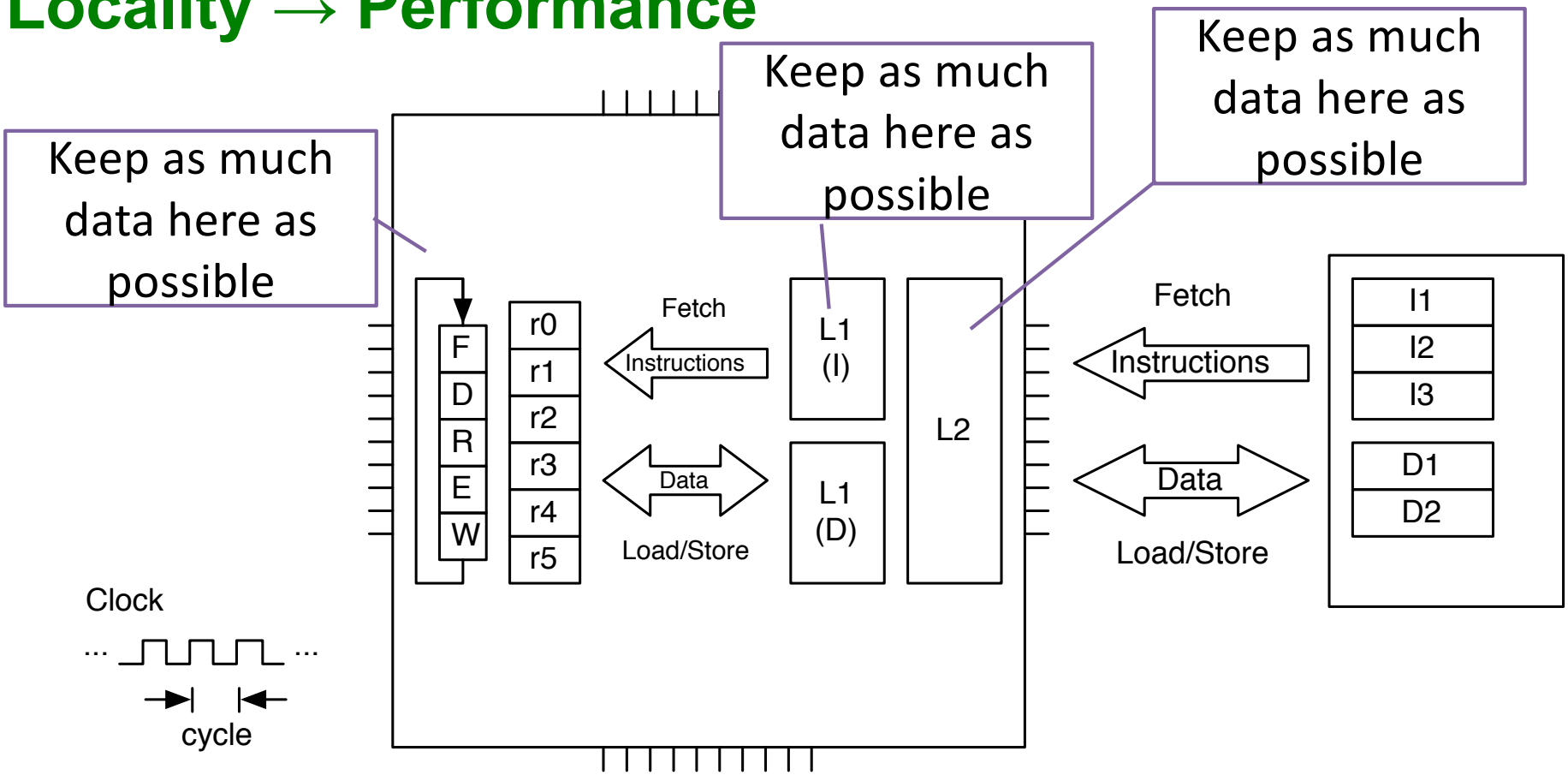
Cache and Multicore



Locality → Strategy



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()

Expressiveness

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

You can write:

```
Matrix A(5, 5), B(5, 5), C(5, 5), D(5,5);
D = A*B + C;
```

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

Benchmarking

```
double benchmark(size_t M, size_t N, size_t K, size_t numruns) {
  Matrix A(M, K), B(K, N), C(M, N);

  Timer T;
  T.start();
  for (size_t i = 0; i < numruns; ++i) {
    multiply(A, B, C);
  }
  T.stop();

  return T.elapsed();
}
```

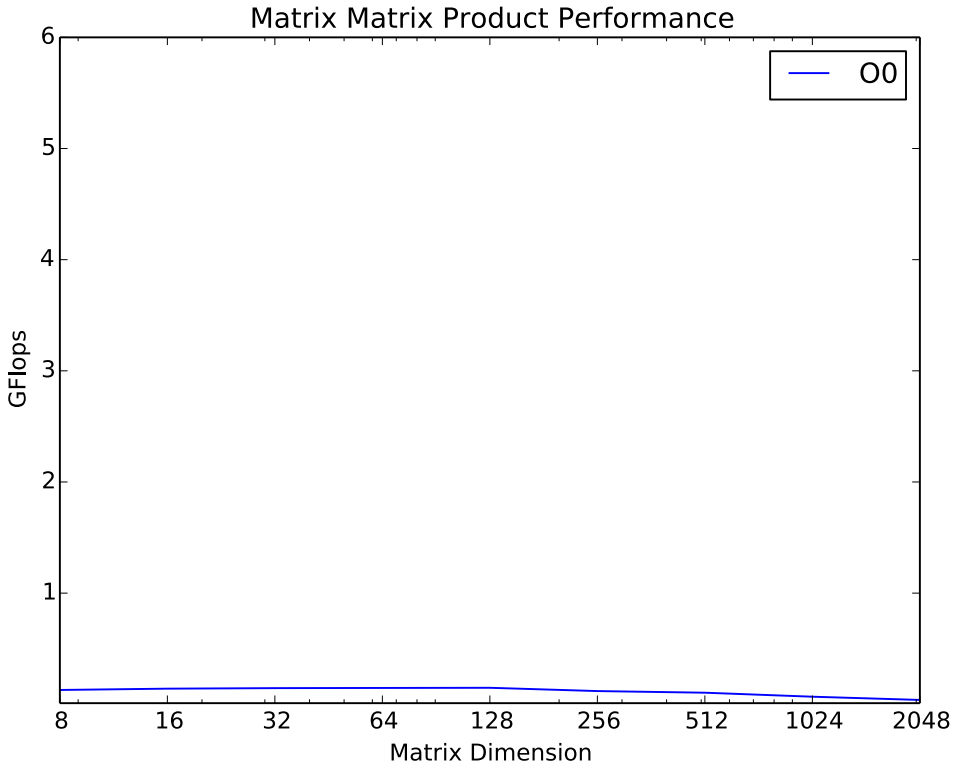
Run the core loop many times to get sufficient resolution for small(er) sizes

Let's Start Benchmarking

```
double benchmark(size_t M, size_t N, size_t K, size_t numruns) {
  Matrix A(M, K), B(K, N), C(M, N);

  Timer T;
  T.start();
  for (size_t i = 0; i < numruns; ++i) {
    multiply(A, B, C);
  }
  T.stop();

  return T.elapsed();
}
```

```
bench: bench.o Matrix.o
c++ -std=c++11 bench.o Matrix.o -o bench

bench.o: bench.cpp Matrix.hpp
c++ -std=c++11 -c bench.cpp -o bench.o

Matrix.o: Matrix.cpp Matrix.hpp
c++ -std=c++11 -c Matrix.cpp -o Matrix.o
```

Base Performance Results



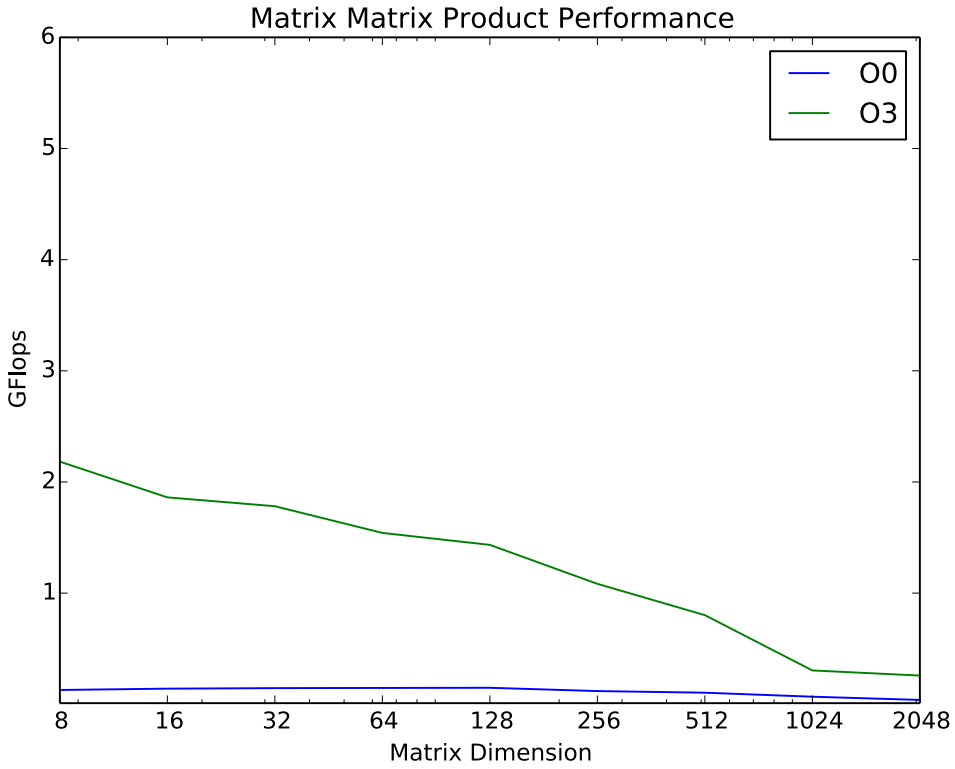
Let's Make One Small Change

```
double benchmark(size_t M, size_t N, size_t K, size_t numruns) {
  Matrix A(M, K), B(K, N), C(M, N);

  Timer T;
  T.start();
  for (size_t i = 0; i < numruns; ++i) {
    multiply(A, B, C);
  }
  T.stop();

  return T.elapsed();
}
```

Tell the compiler to use optimization level 3

```
bench: bench.o Matrix.o
c++ -O3 -std=c++11 bench.o Matrix.o -o bench

bench.o: bench.cpp Matrix.hpp
c++ -O3 -std=c++11 -c bench.cpp -o bench.o

Matrix.o: Matrix.cpp Matrix.hpp
c++ -O3 -std=c++11 -c Matrix.cpp -o Matrix.o
```

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

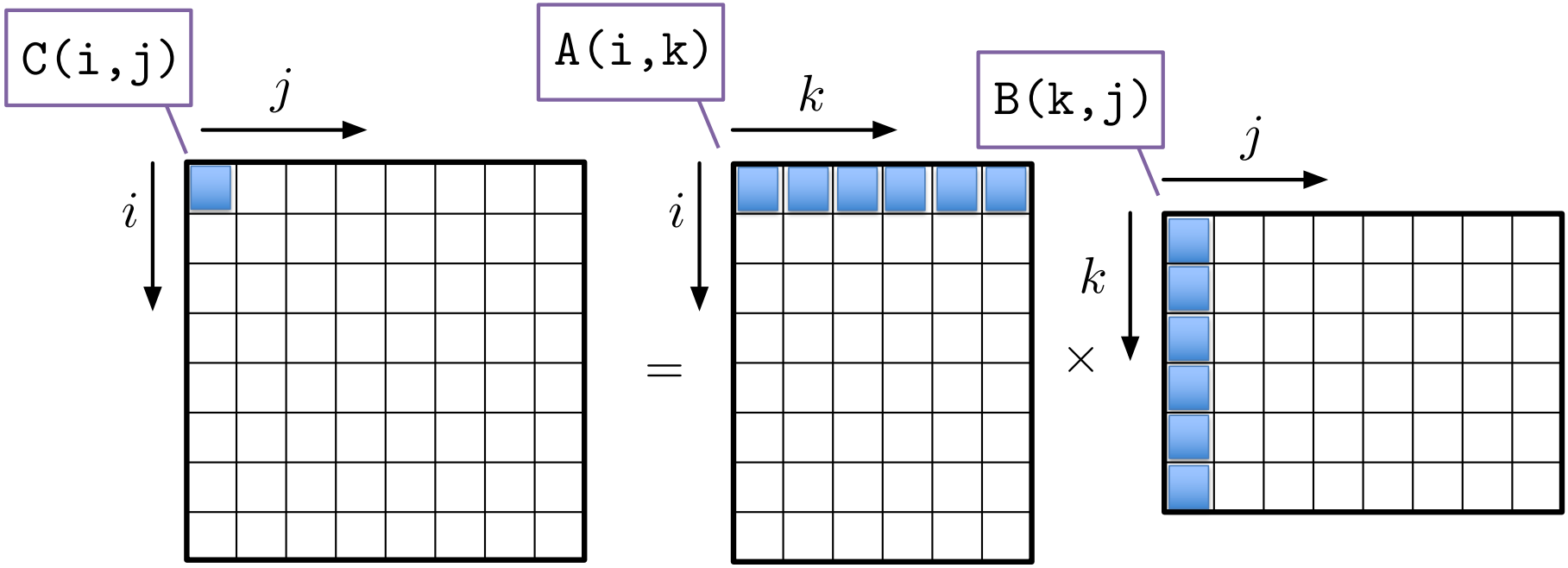
Hoist C(i,j)

```
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;
    }
  }
```

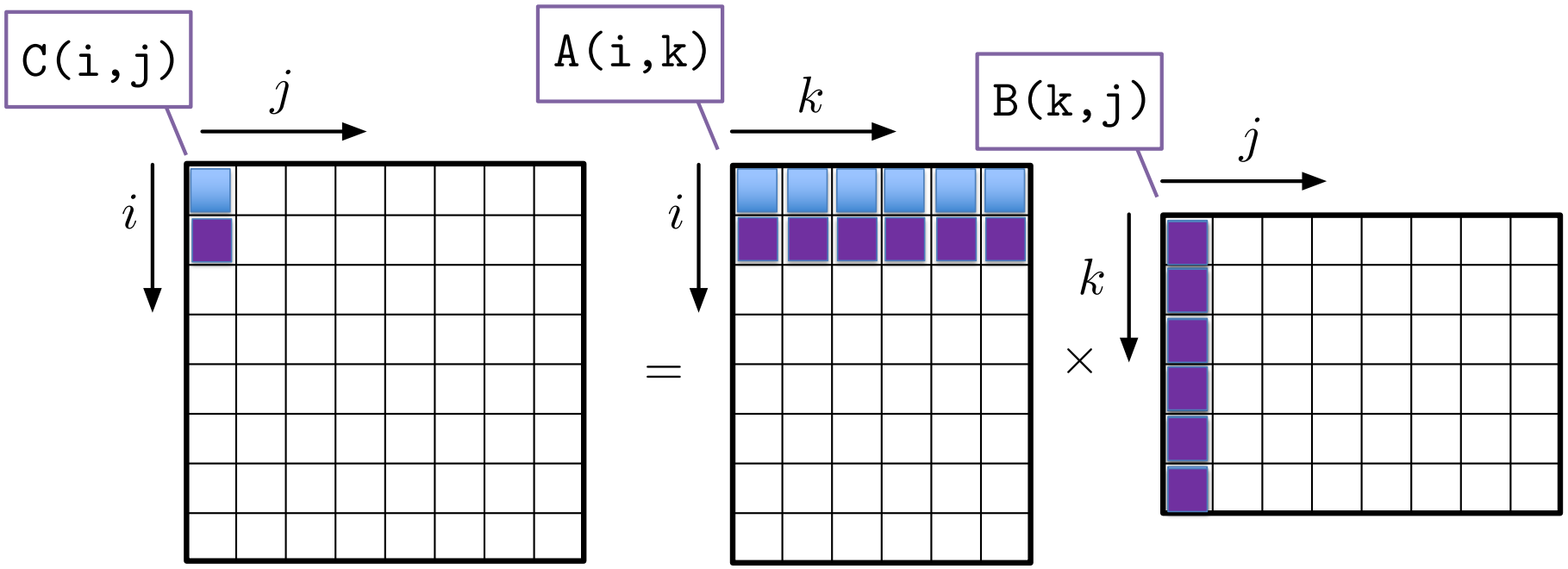
- Load `A(i,k)`
- Load `B(k,j)`
- Multiply
- Add

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

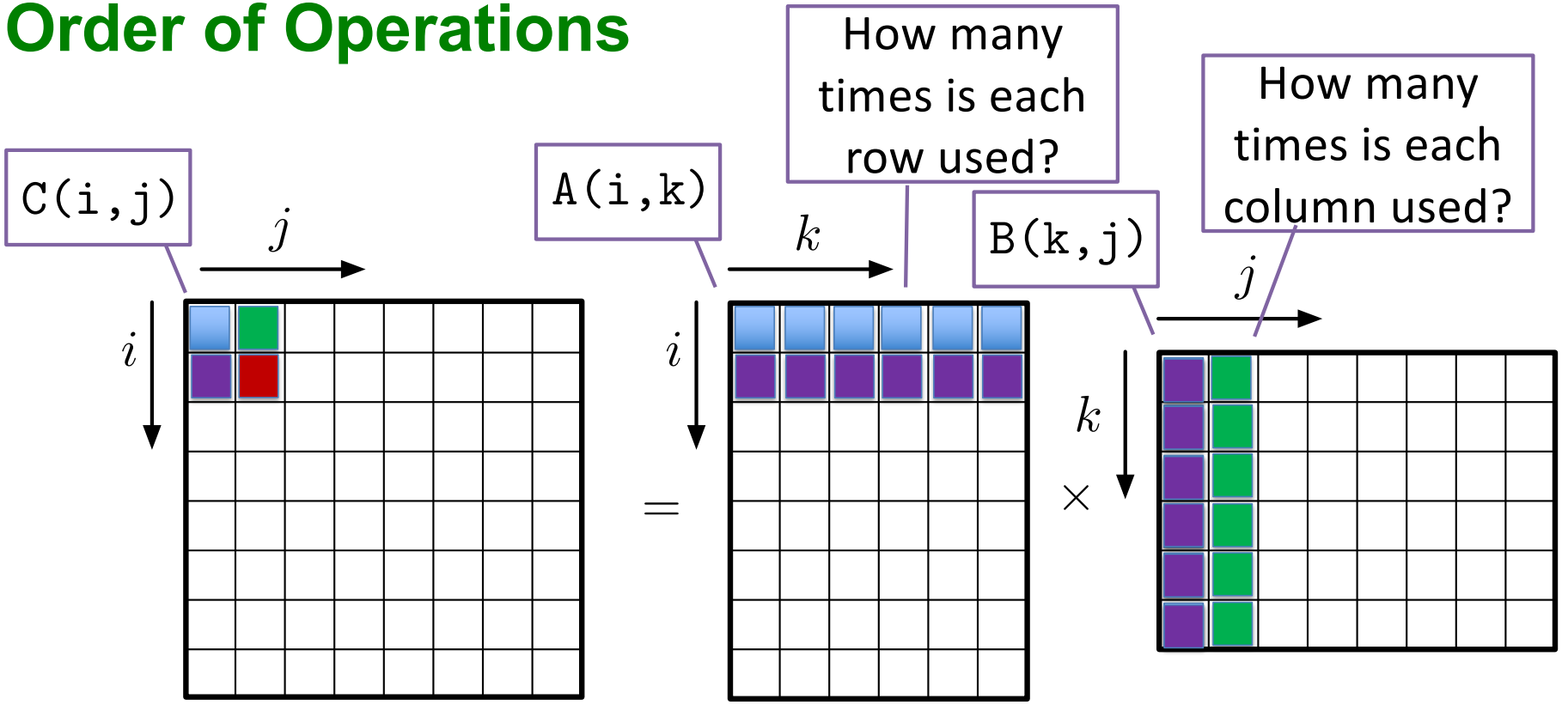
Order of Operations



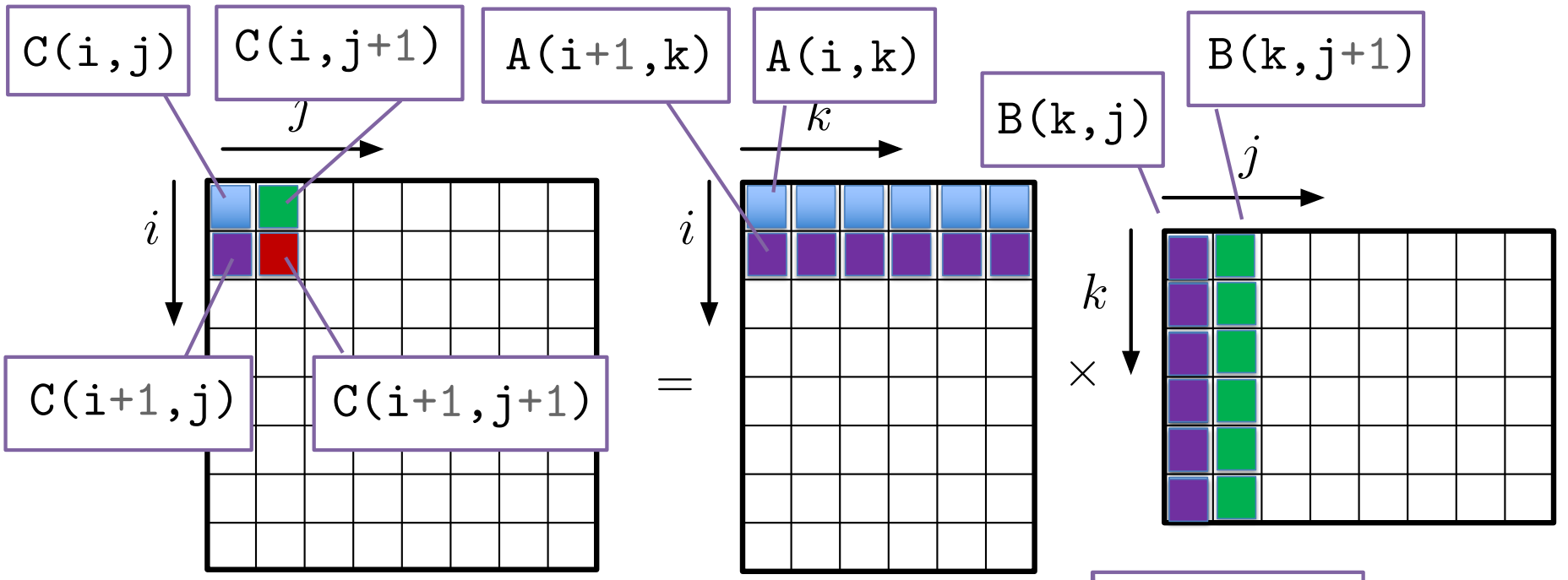
Order of Operations



Order of Operations



Reuse: How Many Times Are Data Reused?



Each is used twice

Improving Locality: Unroll and Ja

```
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

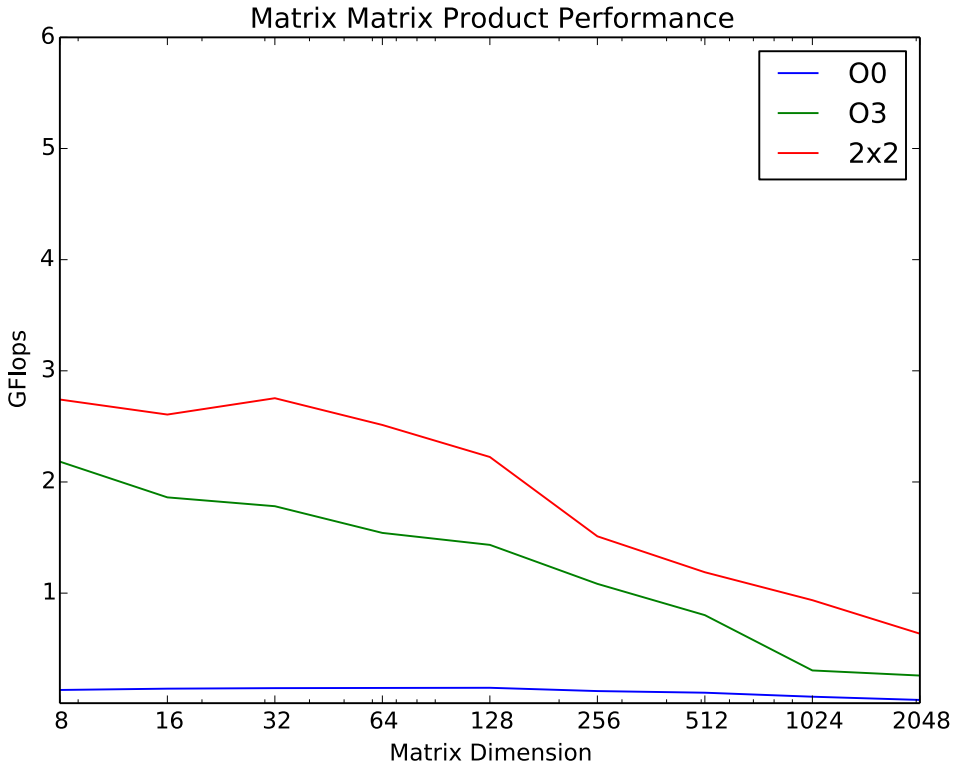
A(i,k) is used twice

Can also hoist (independent of k)

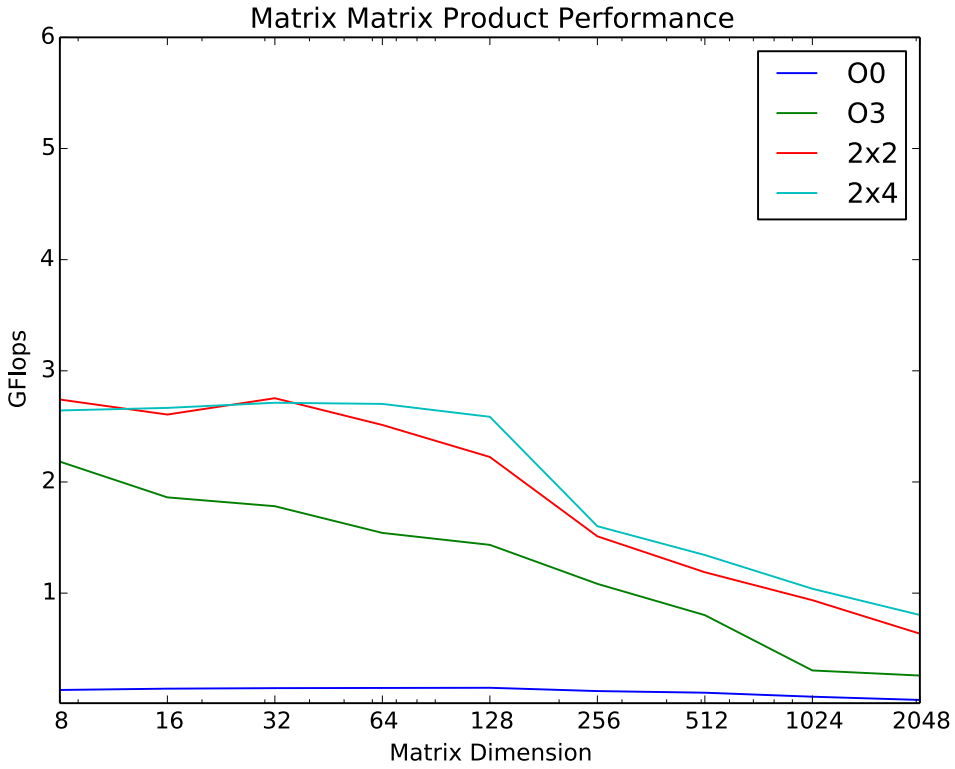
A(i+1,k) is used twice

- 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

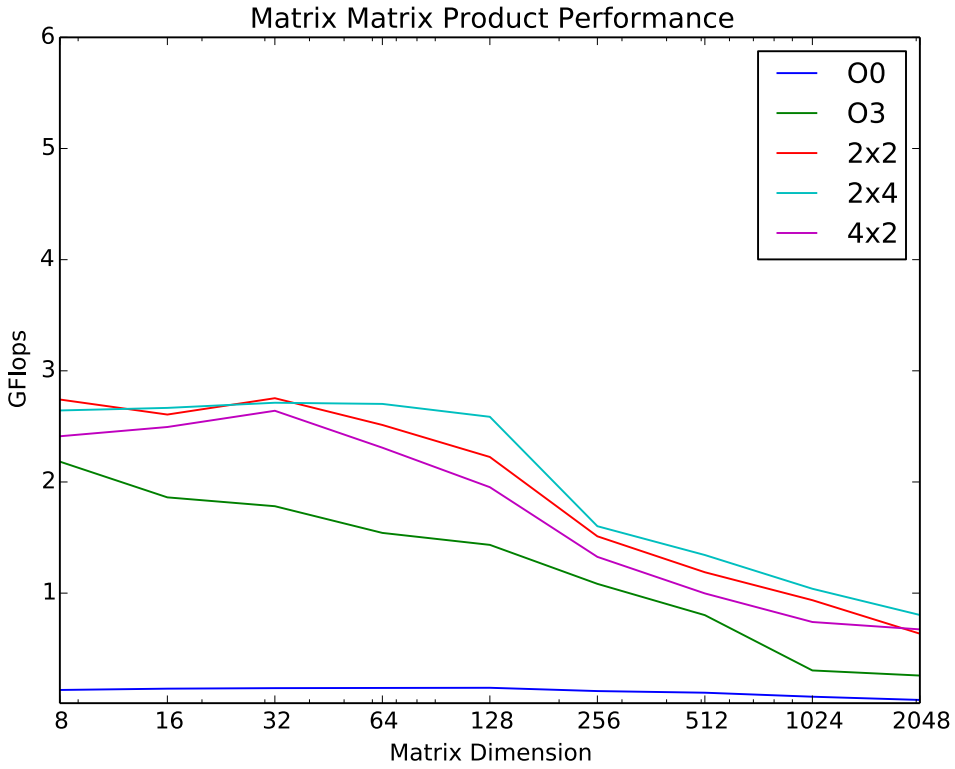
Example: Register Locality



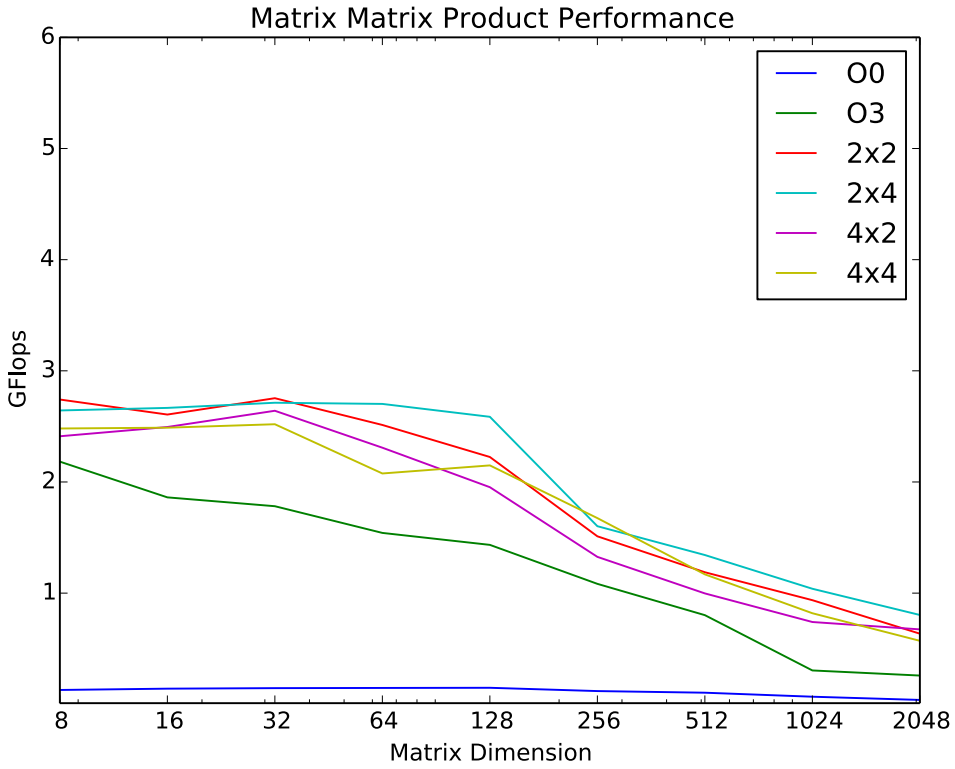
2 by 4


Matrix Matrix Product Performance
GFlops
Matrix Dimension
O0
O3
2x2
2x4
1
2
3
4
5
6
8
16
32
64
128
256
512
1024
2048

4 by 2


Matrix Matrix Product Performance
GFlops
Matrix Dimension
O0
O3
2x2
2x4
4x2
1
2
3
4
5
6
8
16
32
64
128
256
512
1024
2048

4 by 4

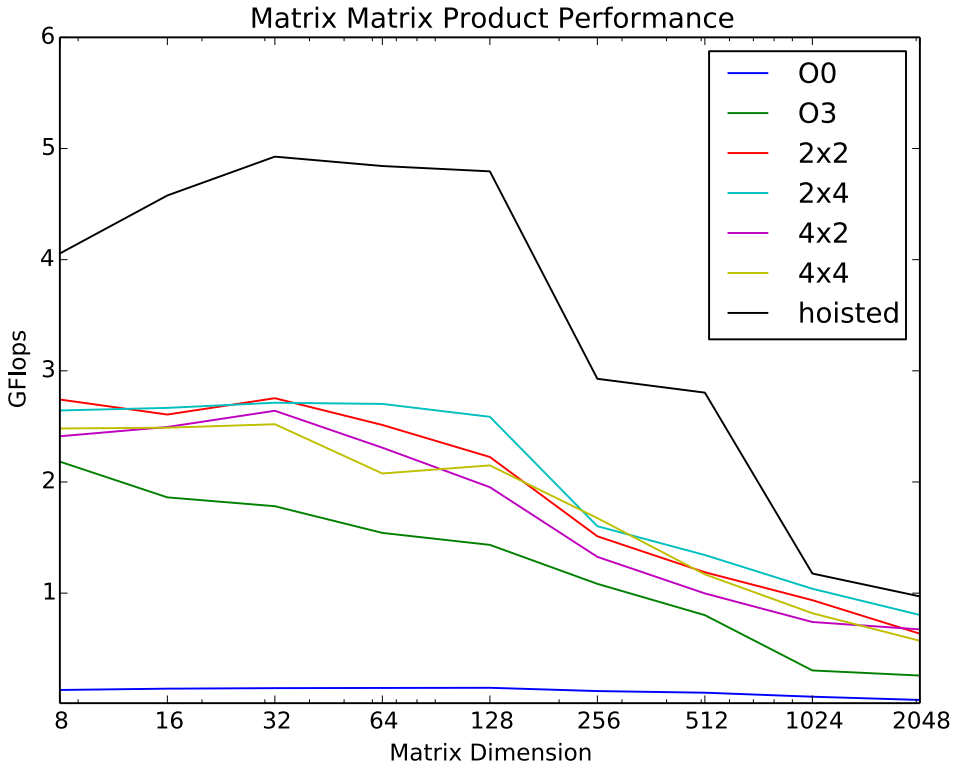

Matrix Matrix Product Performance
GFlops
Matrix Dimension
O0
O3
2x2
2x4
4x2
4x4
1
2
3
4
5
6
8
16
32
64
128
256
512
1024
2048

Tiling and Hoisting

```
void hoistedTiledMultiply2x2(const Matrix& A, const Matrix&B, Matrix&C) {
  for (size_t i = 0; i < A.num_rows(); i += 2) {
    for (size_t j = 0; j < B.num_cols(); j += 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 (size_t k = 0; k < A.num_cols(); ++k) {
            t00 += A(i  , k) * B(k, j  );
            t01 += A(i  , k) * B(k, j+1);
            t10 += A(i+1, k) * B(k, j  );
            t11 += A(i+1, k) * B(k, j+1);
      }
      C(i,  j) = t00;  C(i,  j+1) = t01;
      C(i+1,j) = t10;  C(i+1,j+1) = t11;
    }
  }
}
```

Hoist 2x2 tile

Tiling and Hoisting



Hoisting

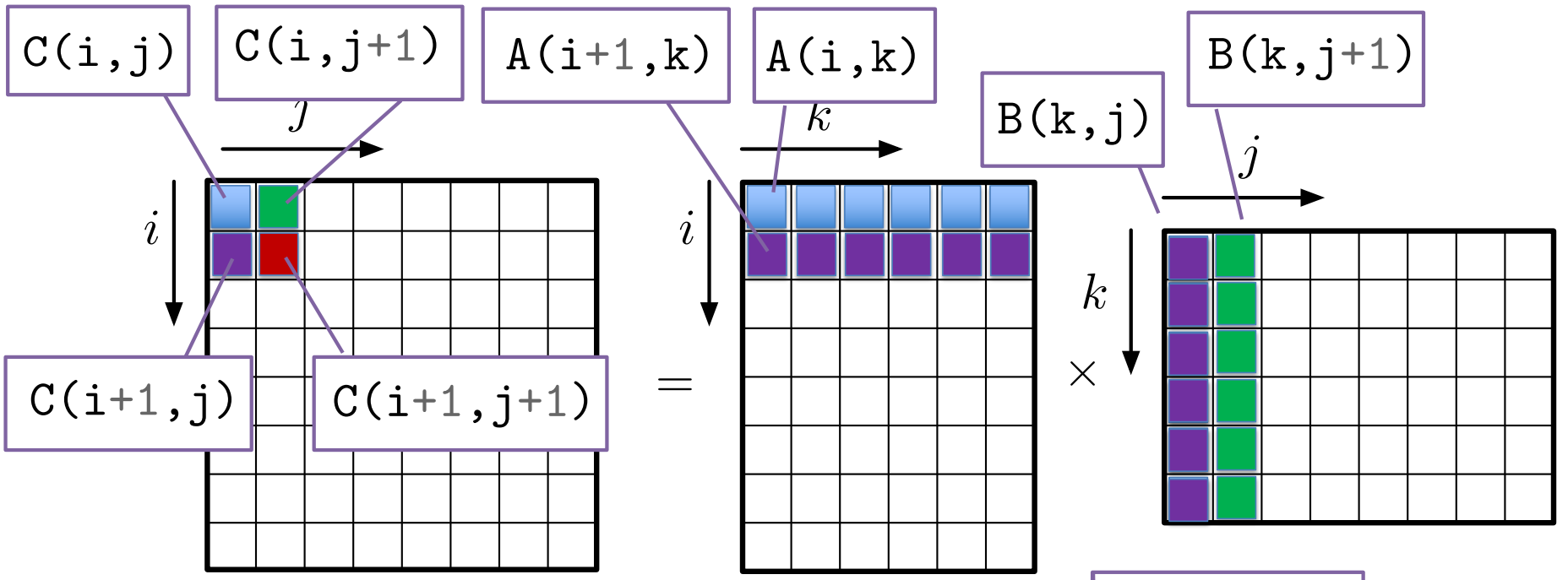
Hoist C(i,j)

```
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;
    }
  }
```

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

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

Reuse: How Many Times Are Data Reused?



Each is used twice

Improving Locality: Unroll and J

```
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

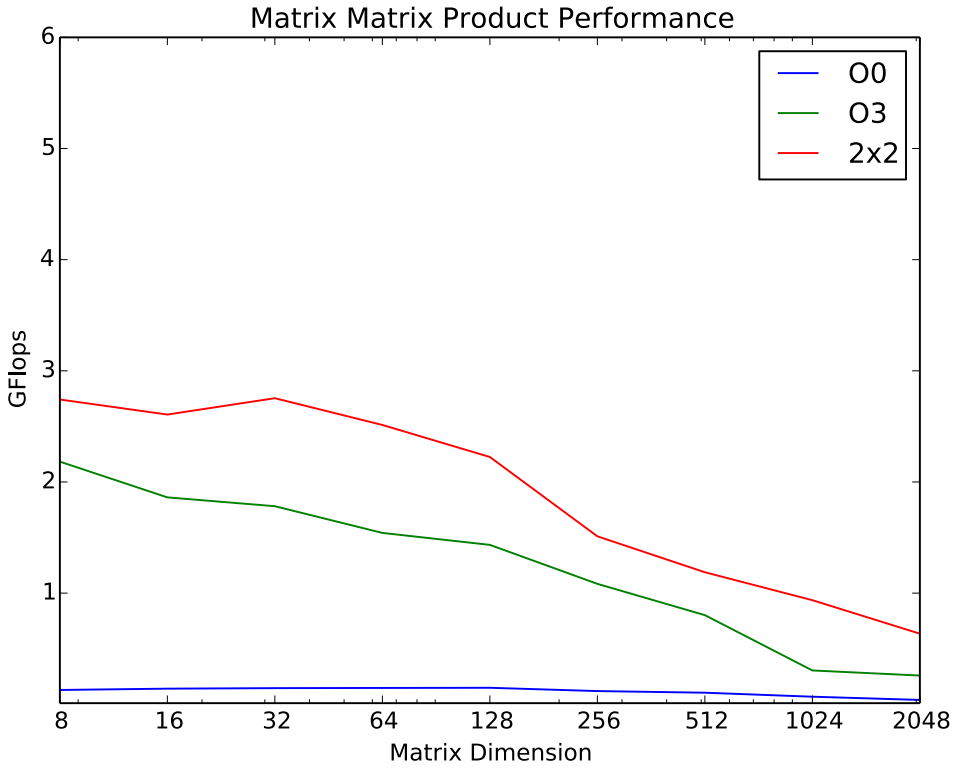
A(i,k) is used twice

Can also hoist (independent of k)

A(i+1,k) is used twice

- 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

Example: Register Locality

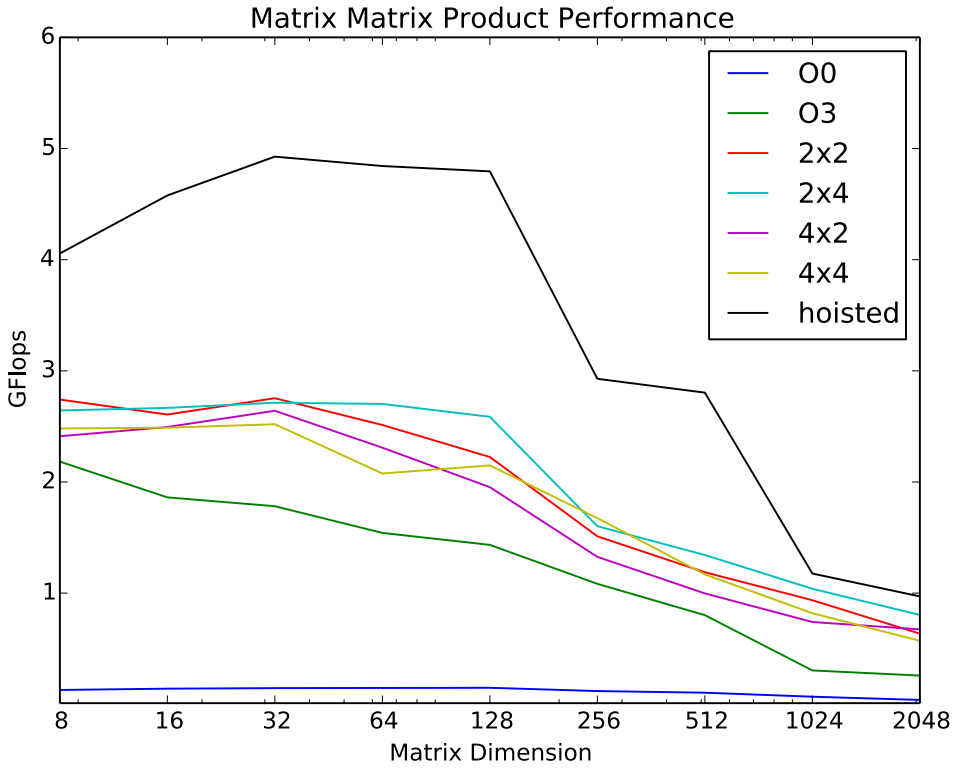


Tiling and Hoisting

```
void hoistedTiledMultiply2x2(const Matrix& A, const Matrix& B, Matrix& C) {
  for (size_t i = 0; i < A.num_rows(); i += 2) {
    for (size_t j = 0; j < B.num_cols(); j += 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 (size_t k = 0; k < A.num_cols(); ++k) {
        t00 += A(i  , k) * B(k, j  );
        t01 += A(i  , k) * B(k, j+1);
        t10 += A(i+1, k) * B(k, j  );
        t11 += A(i+1, k) * B(k, j+1);
      }
      C(i,  j) = t00;  C(i,  j+1) = t01;
      C(i+1,j) = t10;  C(i+1,j+1) = t11;
    }
  }
}
```

Hoist 2x2 tile

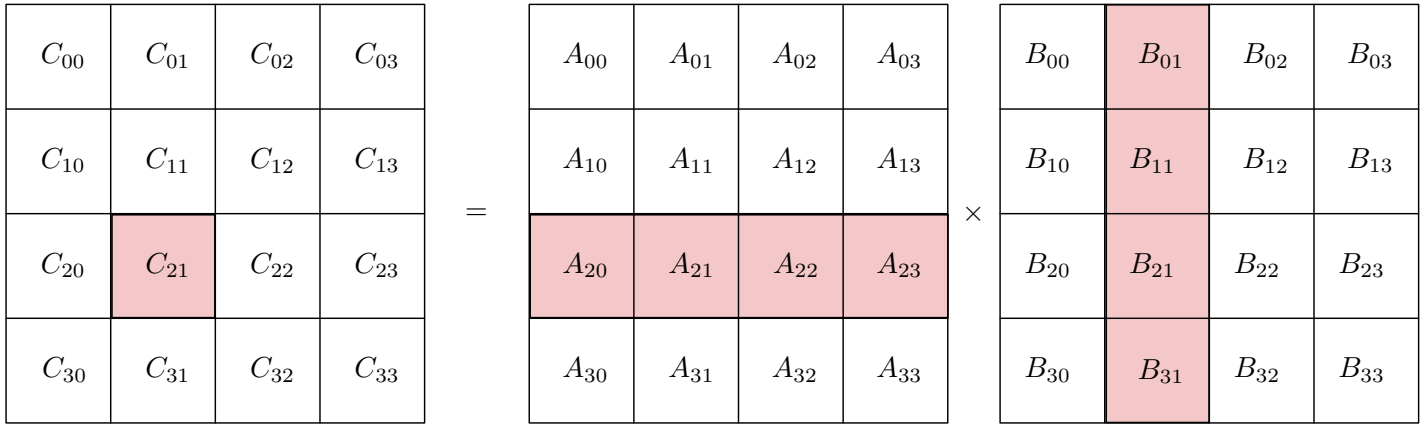
Tiling and Hoisting



Improving Locality: Cache

- Large matrix problems won't fit completely into cache
- Use blocked algorithm – work with blocks that will fit into cache

$$C_{IJ} = \sum_K A_{IK} B_{KJ}$$



$$C_{21} = A_{20}B_{01} + A_{21}B_{11} + A_{22}B_{21} + A_{23}B_{31}$$

- Each product term fits completely into cache and runs at high-performance
- Cache misses amortized — work with $O(N^3)$ data $O(N^2)$

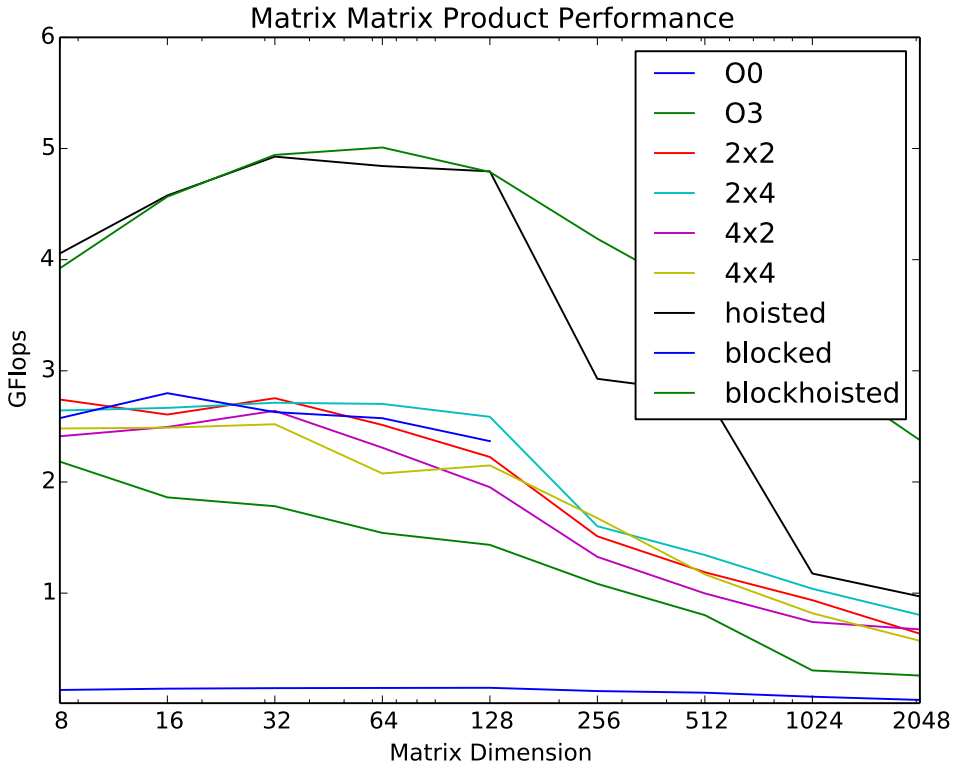
Blocking and Tiling

```
void blockedTiledMultiply2x2(const Matrix& A, const Matrix& B, Matrix& C) {
  const int blocksize = std::min(A.num_rows(), 32);

  for (size_t ii = 0; ii < A.num_rows(); ii += blocksize) {
    for (size_t jj = 0; jj < B.num_cols(); jj += blocksize) {
      for (size_t kk = 0; kk < A.num_cols(); kk += blocksize) {

        for (size_t i = ii; i < ii+blocksize; i += 2) {
          for (size_t j = jj; j < jj+blocksize; j += 2) {
            for (size_t k = kk; k < kk+blocksize; ++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);
            }
          }
        }
      }
    }
  }
}
```

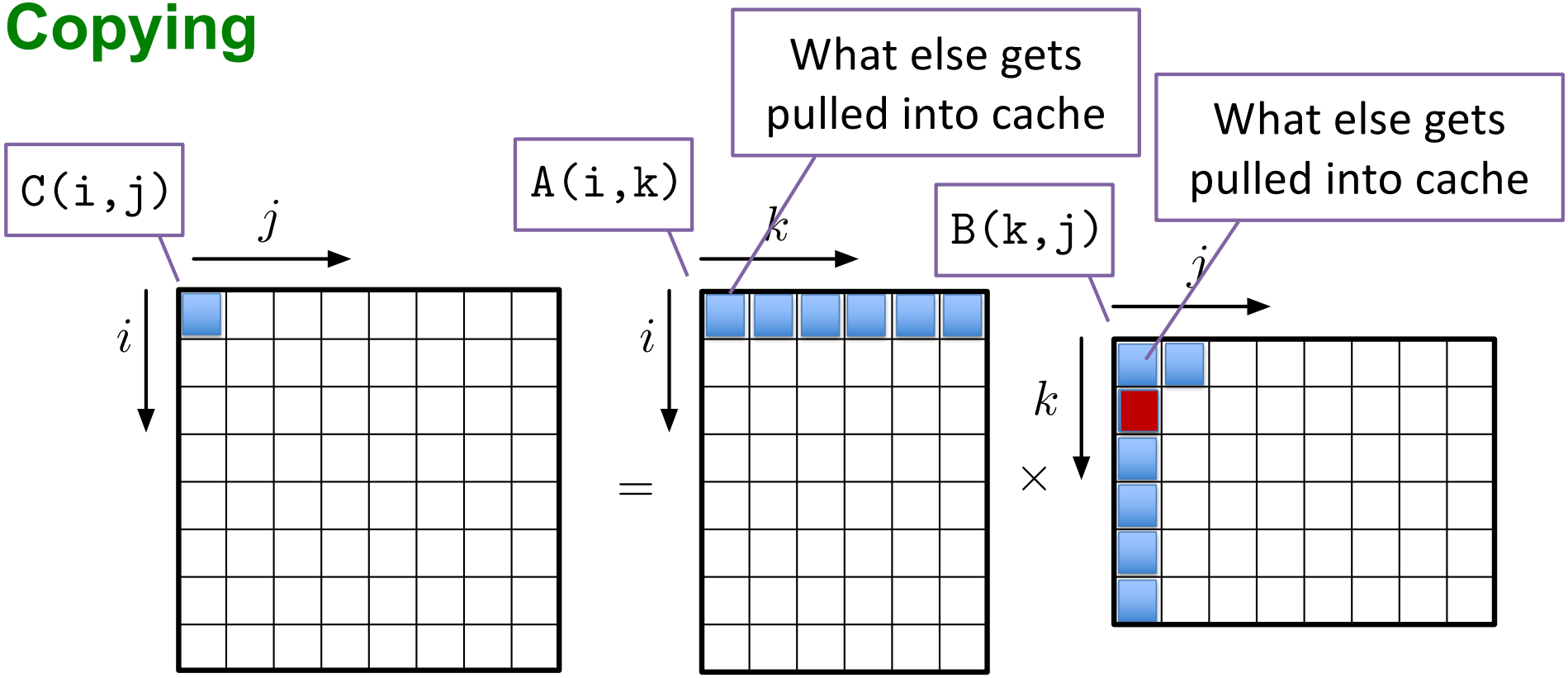
Outer loops work across blocks (for each block)

Inner loops work on blocks

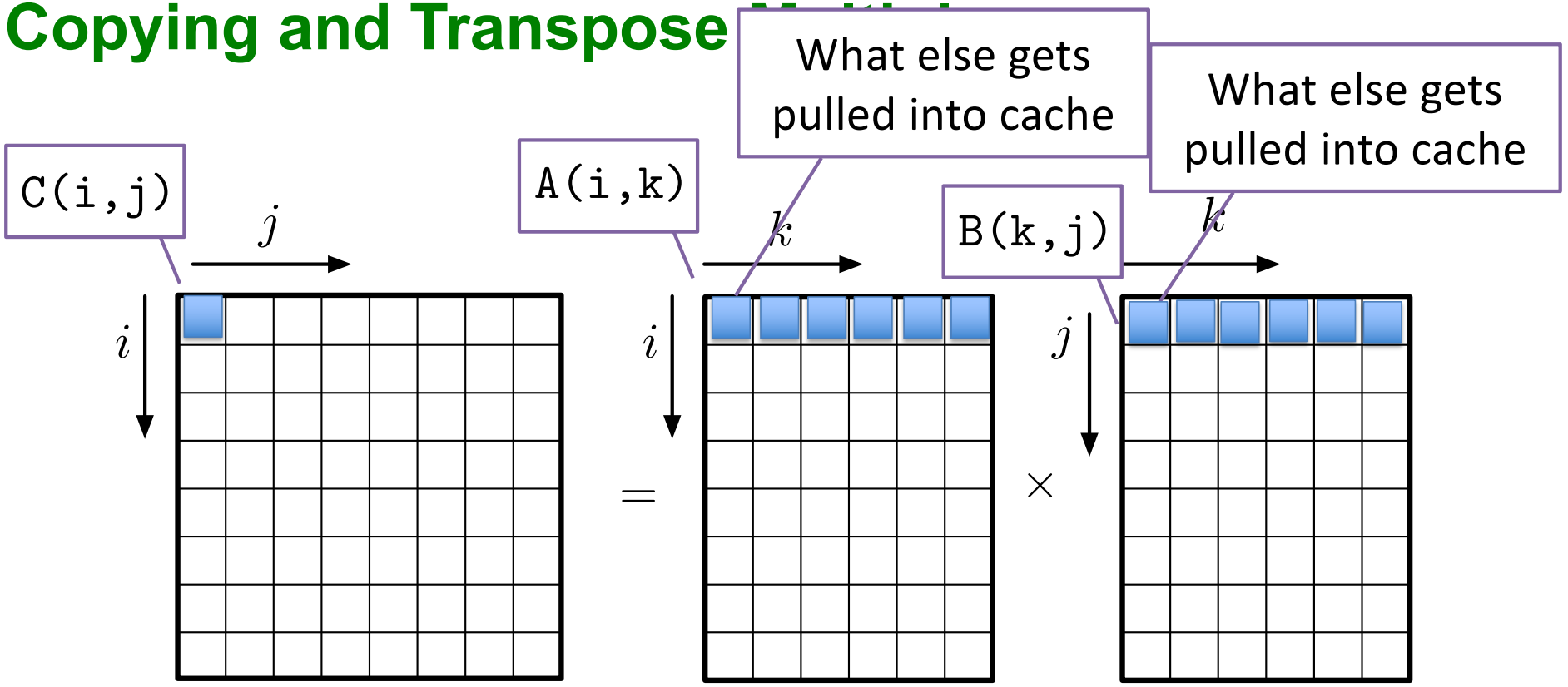
Blocking and Tiling and Hoisting



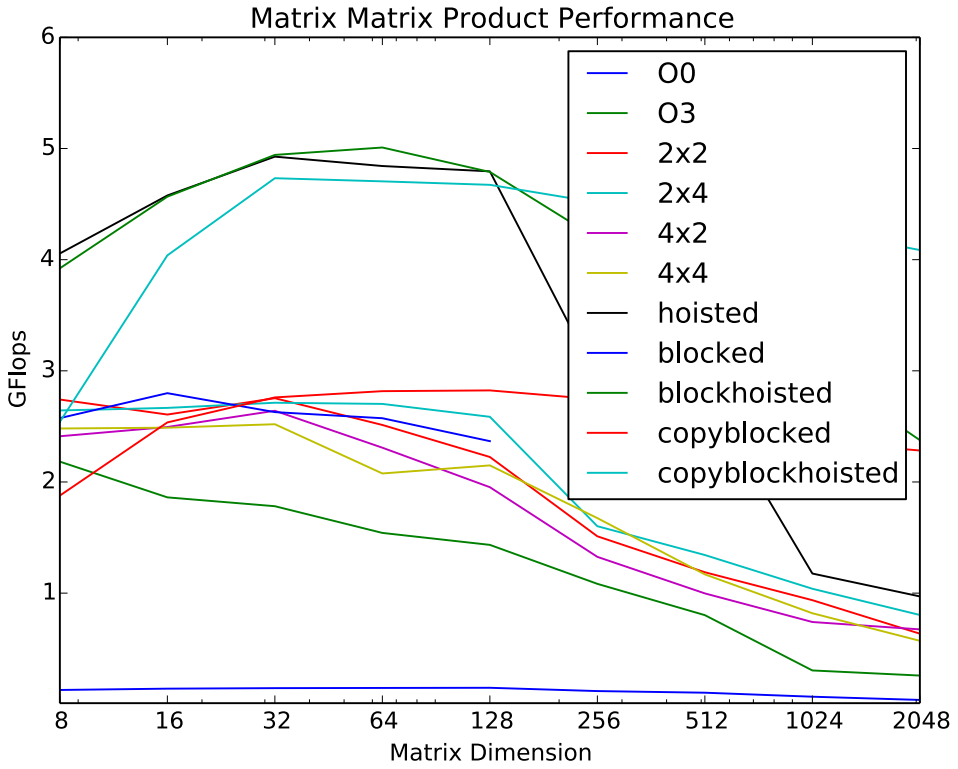
Copying


C(i,j)
A(i,k)
B(k,j)
What else gets pulled into cache
What else gets pulled into cache
i
j
i
k
=
k
×
j

Copying and Transpose



Blocking and Tiling and Hoisting and Copying



Tuning

How do we find the optimal combination?

Magic: the power of apparently influencing the course of events by using mysterious or supernatural forces

- Starting with base code
- Various compiler optimizations help
- Tiling (which size)
- Blocking (what size)
- What size works best for Tiling and Blocking ***together?***

- What loop ordering? Matrix matrix product has six different orderings? What block ordering?

- What about when we add AVX, and threads, etc?

The answer will be different for different CPUs

Finding the Sweet Spot

- Exhaustive parameter space search
  - Tiling, Blocking, Compiler flags, AVX inst, loop ordering
- Original project at UC Berkeley phiPAC (Bilmes et al)
- Further developed by Whaley and Dongarra → Automatically Tuned Linear Algebra Subprograms (ATLAS)
  - Recently honored with "test of time" award
- (cf) also "Goto" BLAS and FLAME (Goto, van de Geijn)

And wrote a program to generate different multiply functions

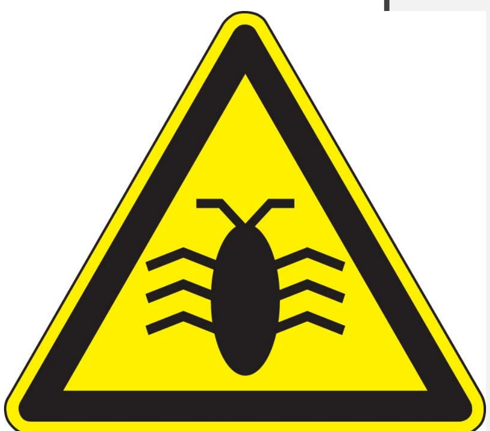
This started as a final course project

The competition was to write fastest matrix-matrix product

Students were the good kind of lazy

One Gigantic Bug

What if num_rows is not an integer product of blocksize?



```
void blockedTiledMultiply2x2(const Matrix& A, const Ma
  const int blocksize = std::min(A.numRows(), 32);

  for (int ii = 0; ii < A.numRows(); ii += blocksize)
    for (int jj = 0; jj < B.numCols(); jj += blocksiz
      for (int kk = 0; kk < A.numCols(); kk += blocksize) {

        for (int i = ii; i < ii+blocksize; i += 2) {
          for (int j = jj; j < jj+blocksize; j += 2) {
            for (int k = kk; k < kk+blocksize; ++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);
            }
          }
        }
        for (int i = ii; i < ii+blocksize; ++i) {
          for (int j = jj; j < jj+blocksize; ++j) {
            for (int k = kk; k < kk+blocksize; ++k) {
              C(i  , j  ) += A(i  , k) * B(k, j  );
            }
          }
        }
        for (int i = ii; i < ii+blocksize; ++i) {
          for (int j = jj; j < jj+blocksize; ++j) {
            for (int k = kk; k < kk+blocksize; ++k) {
              C(i  , j  ) += A(i  , k) * B(k, j  );
            }
          }
        }
        for (int i = ii; i < ii+blocksize; ++i) {
          for (int j = jj; j < jj+blocksize; ++j) {
            for (int k = kk; k < kk+blocksize; ++k) {
              C(i  , j  ) += A(i  , k) * B(k, j  );
            }
          }
        }
      }
    }
  }
}
```

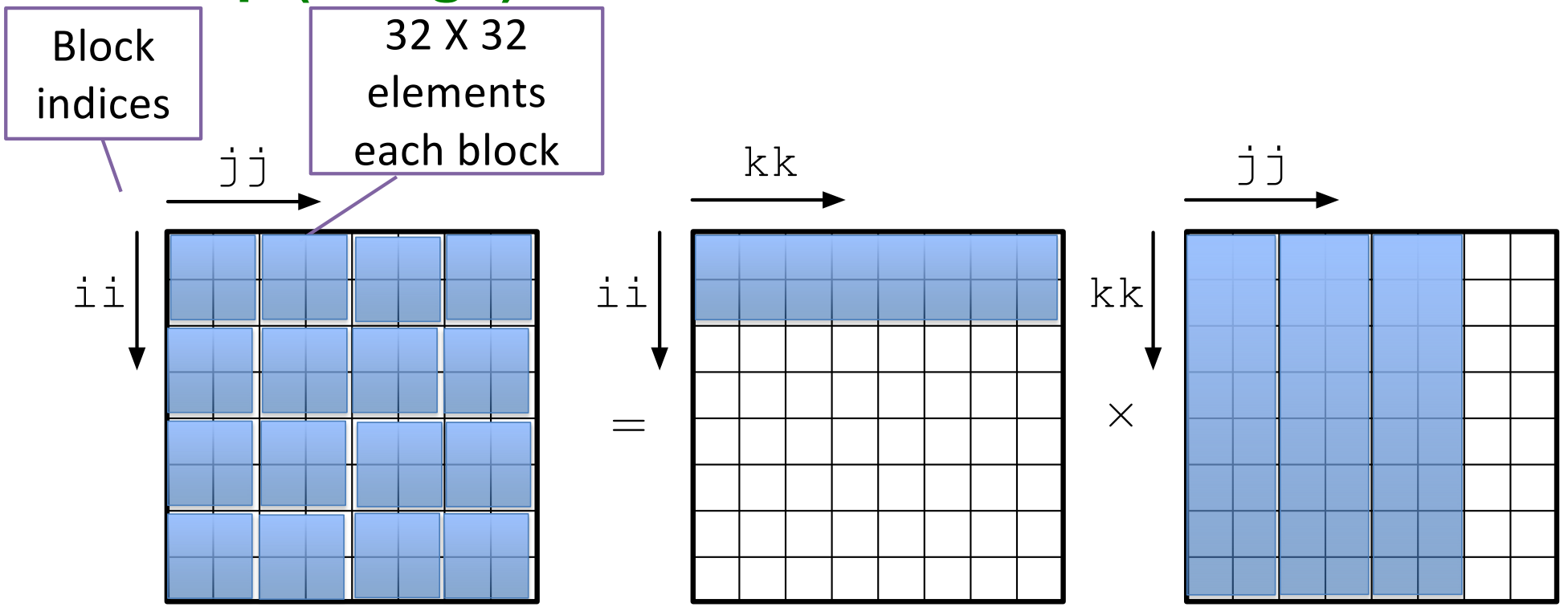
For illustrative purposes only

Example code (slides and source) omit this

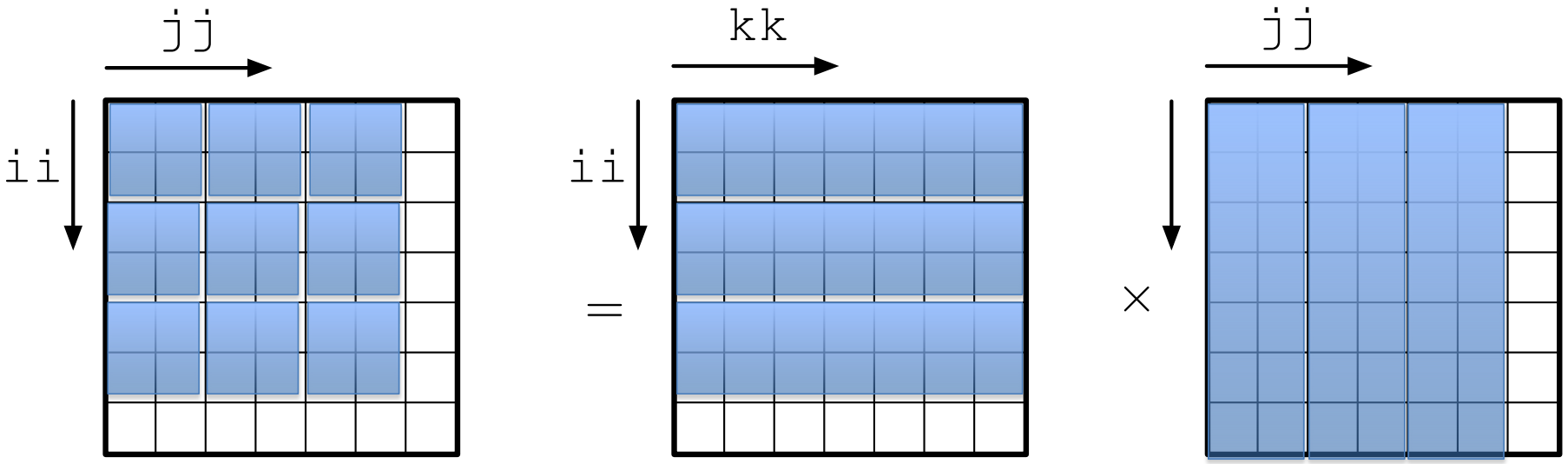
Caveat codor

Powers of 2 are great

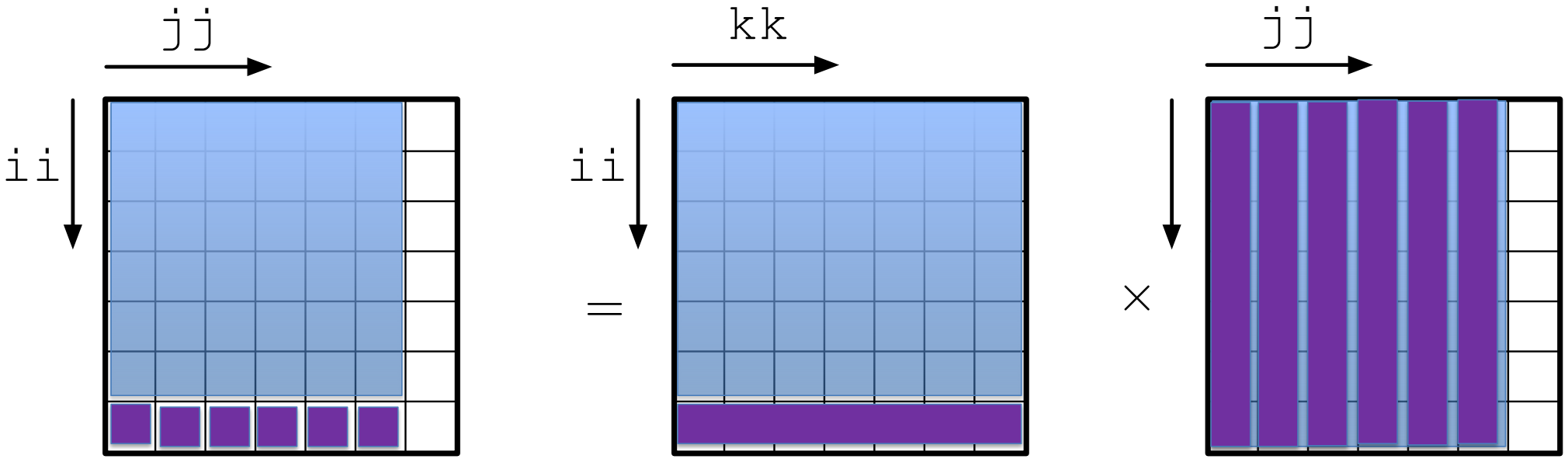
Cleanup (Fringe)



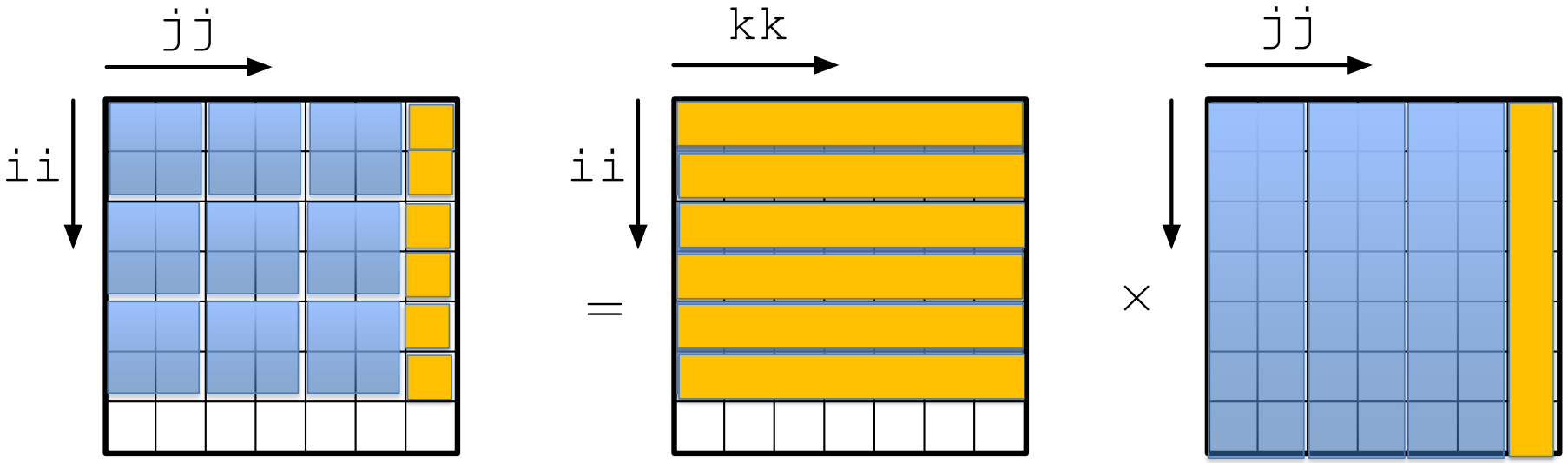
Fringe Cleanup



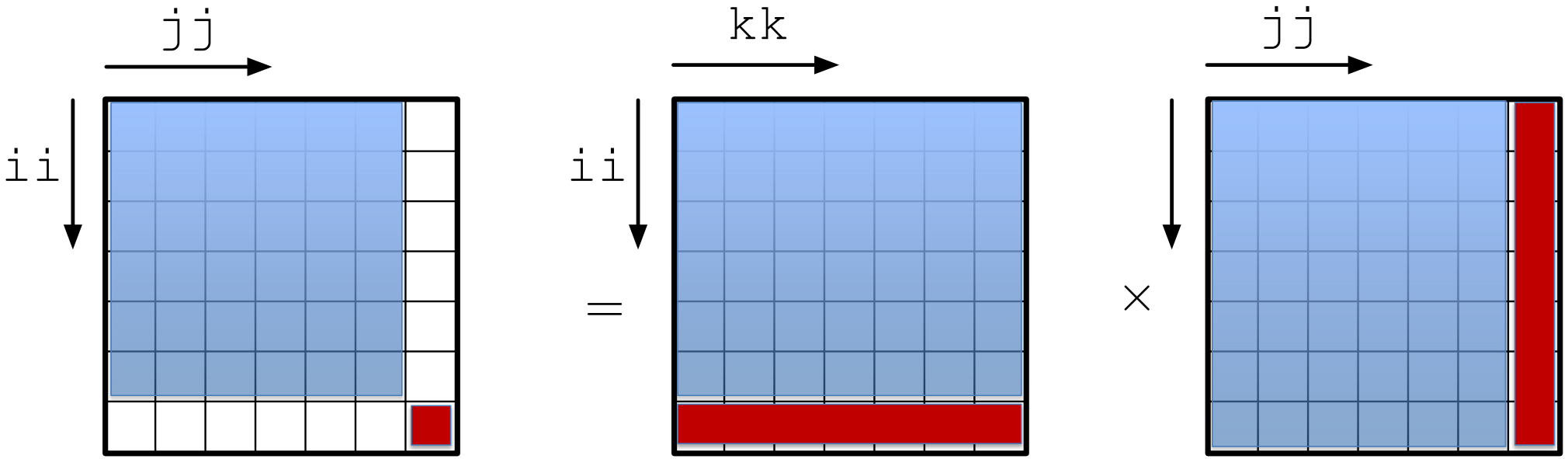
Fringe Cleanup



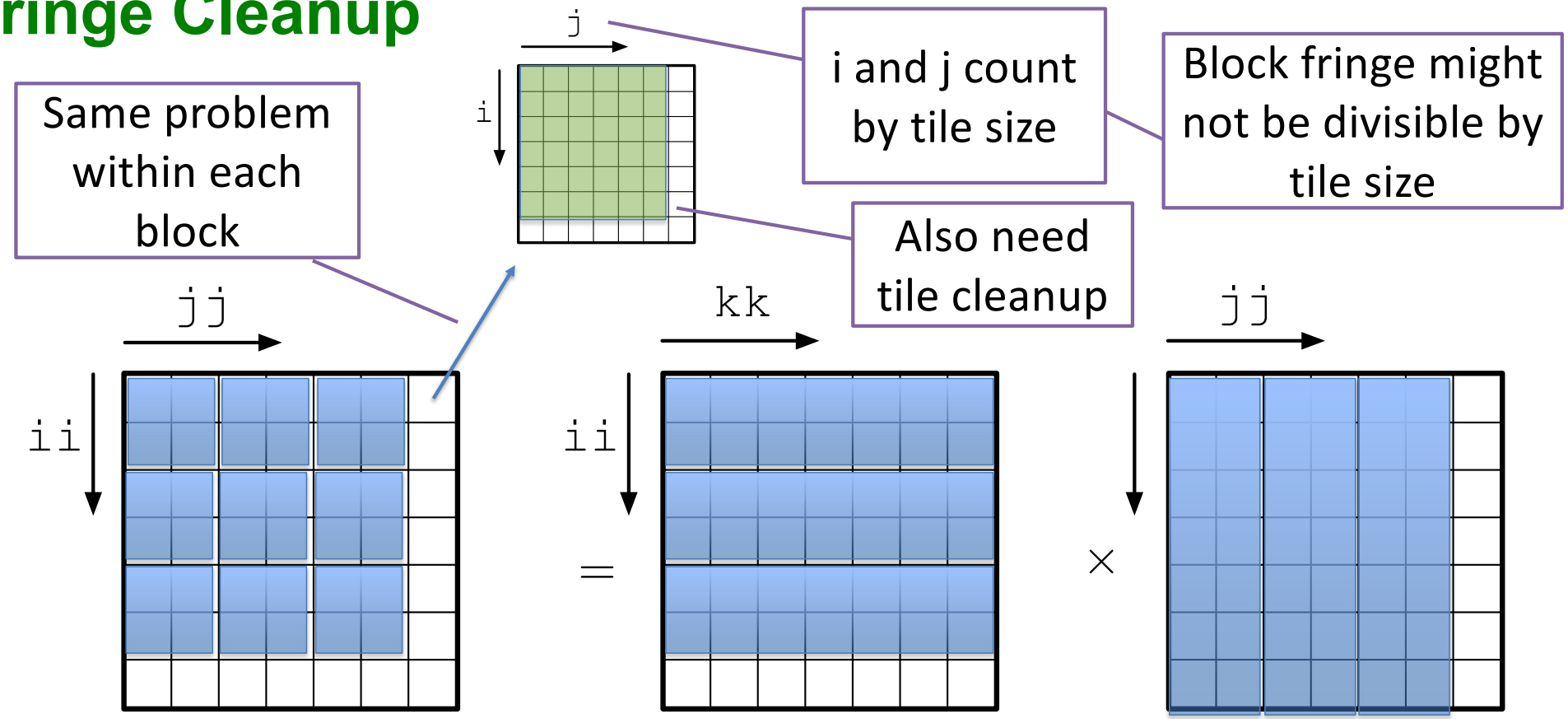
Fringe Cleanup



Fringe Cleanup



Fringe Cleanup

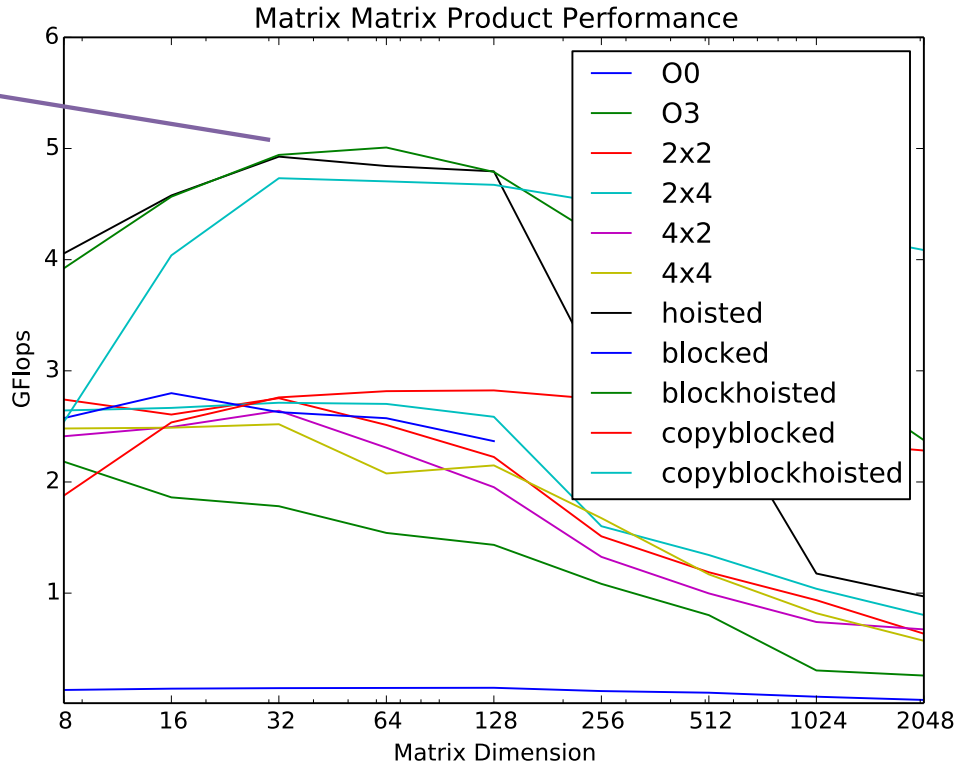


Blocking and Tiling and Hoisting and Copying

Is this the best we can do?

How good is it anyway?

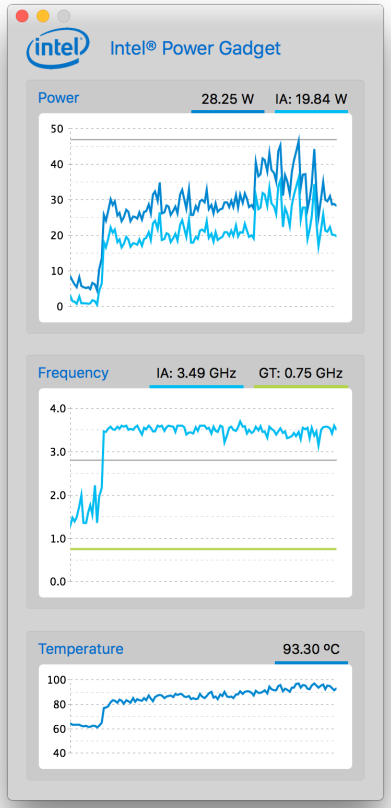
(cf PS 4A)

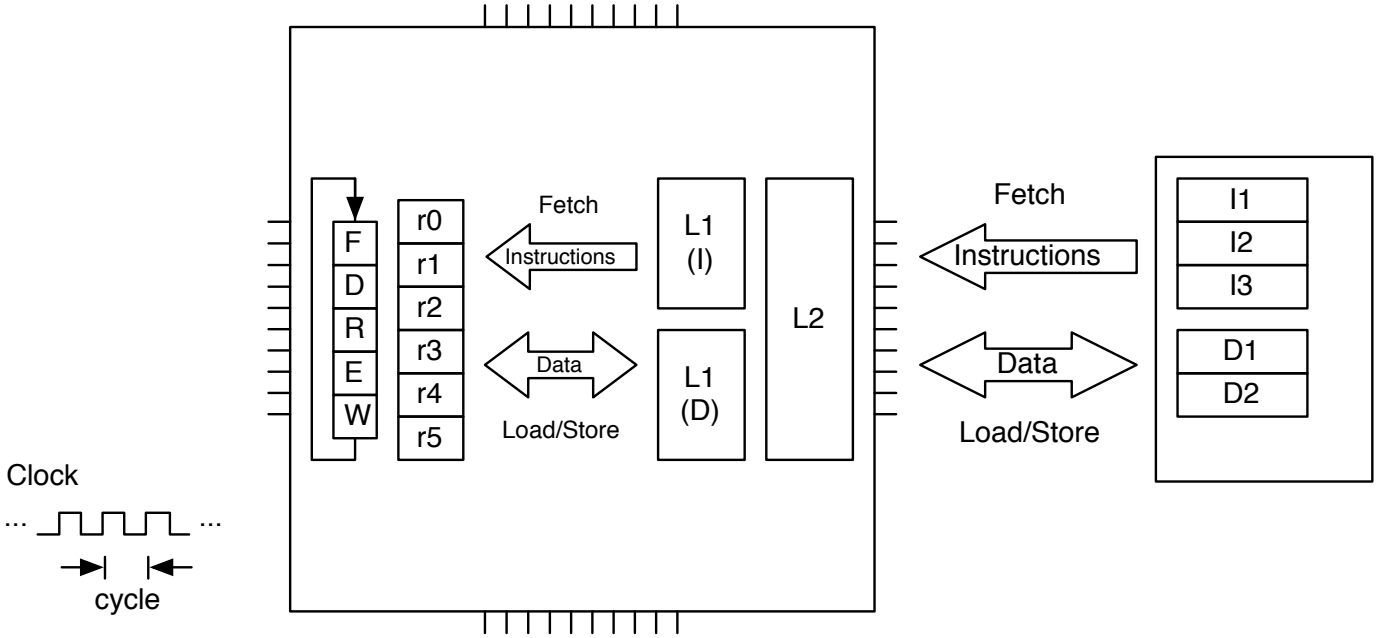


Calypso

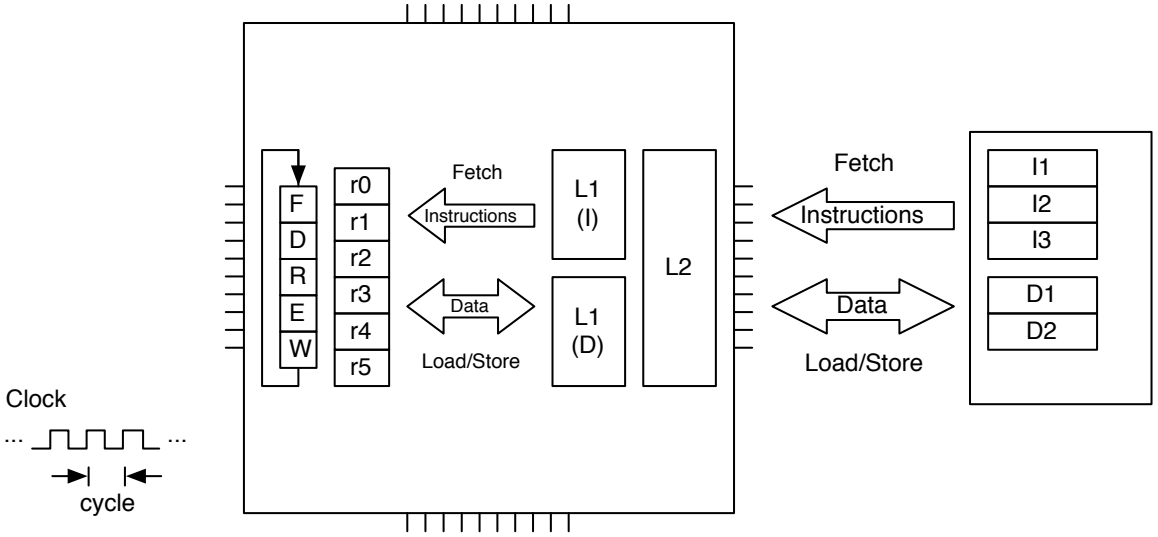
- Program for generating matrix-matrix products

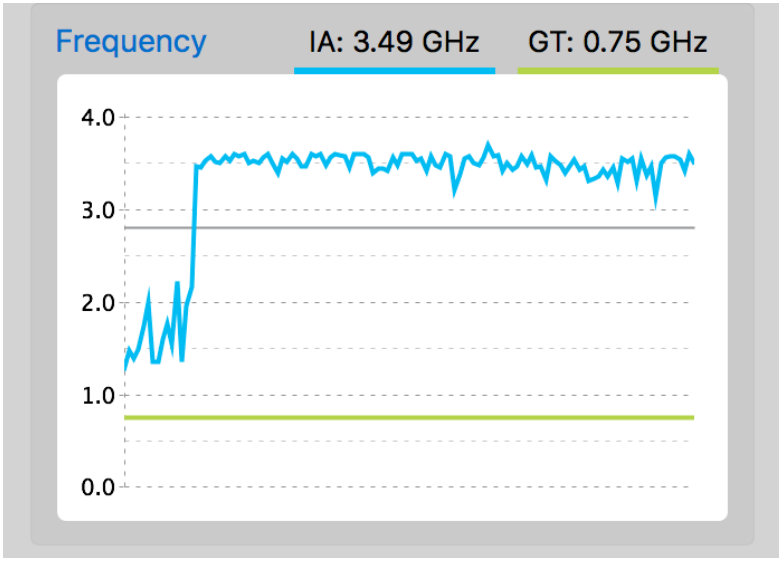
CPU Clock Speed





Peak Performance vs Achieved Performance





$$5 \times 10^9 \frac{\text{FLOPS}}{\text{second}} \div 3.5 \times 10^9 \frac{\text{cycles}}{\text{second}} \approx 1.5 \frac{\text{FLOPS}}{\text{cycle}}$$

Does this make sense?

Science

- Frank Harary once suggested the law that **any field that had the word "science" in its name was guaranteed thereby not to be a science.** He would cite as examples Mxxxxx Science, Lxxxxx Science, Pxxxxxx Science, Hxxxxxxxx Science, Sxxxx Science, and **Computer Science**.

License: Creative Commons 3 - CC BY-SA 3.0
Creator attribution: Nick Youngson - link to - http://nyphotographic.com/
Date first licensed: December 2015
Original Image: http://www.thebluediamondgallery.com/tablet/c/computer-science.html

But is it Science?

"the pursuit and application of knowledge and understanding of the natural and social world following a systematic methodology based on evidence."

"Data on how much of the scientific literature is reproducible are rare and generally bleak."

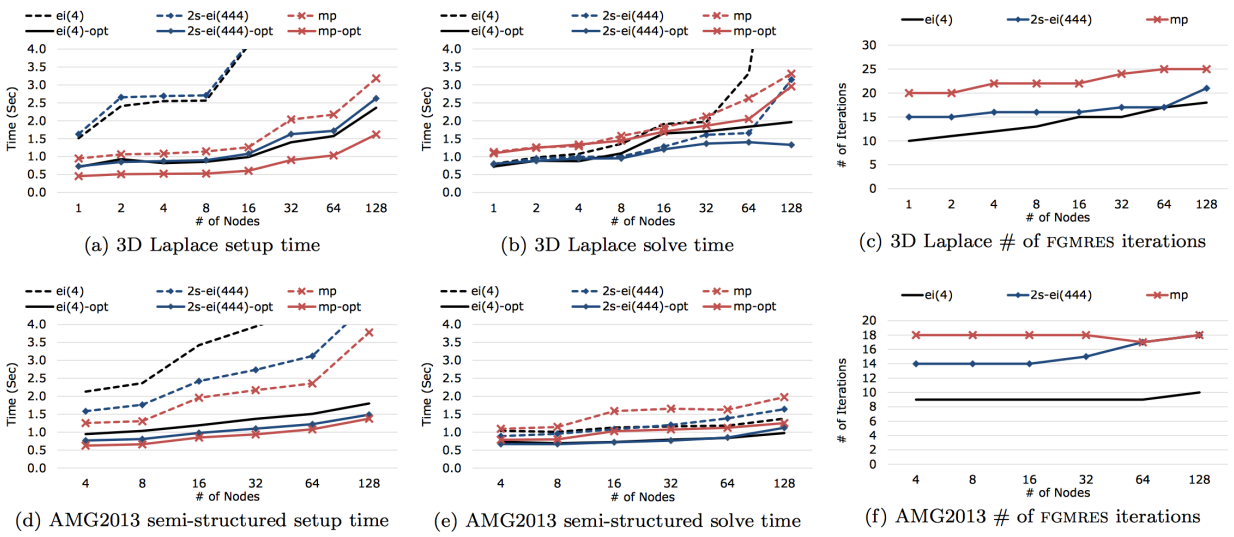
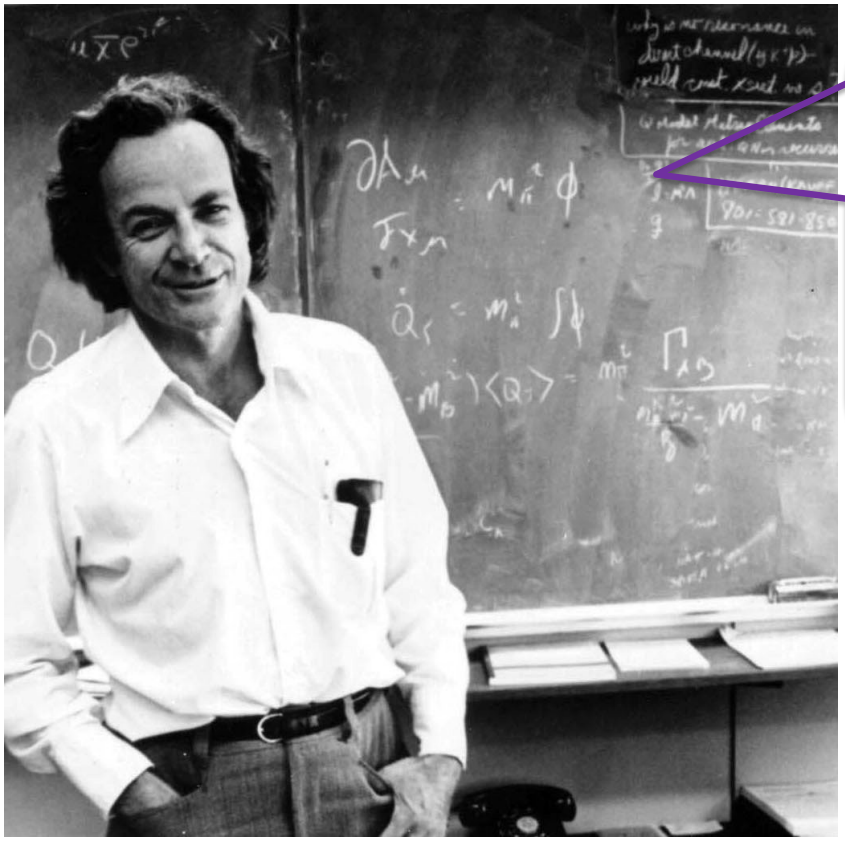


Figure 6: Weak scaling multi-node performance (a-c) 3D Laplace matrix with 27-pt discretization from HPCG benchmark [33], ~27 non-zeros per row, $96^3 \simeq 0.9$M rows and ~0.27 GB per rank. (d-e) The semi-structured input from AMG2013 benchmark [35], r=32 and pooldist=1 (generates realistic inputs and requires ≥8 ranks), ~8 non-zeros per row, ~1.6M rows and 0.15 GB per rank. The reported times are the maximum among ranks.

Name This Famous Person



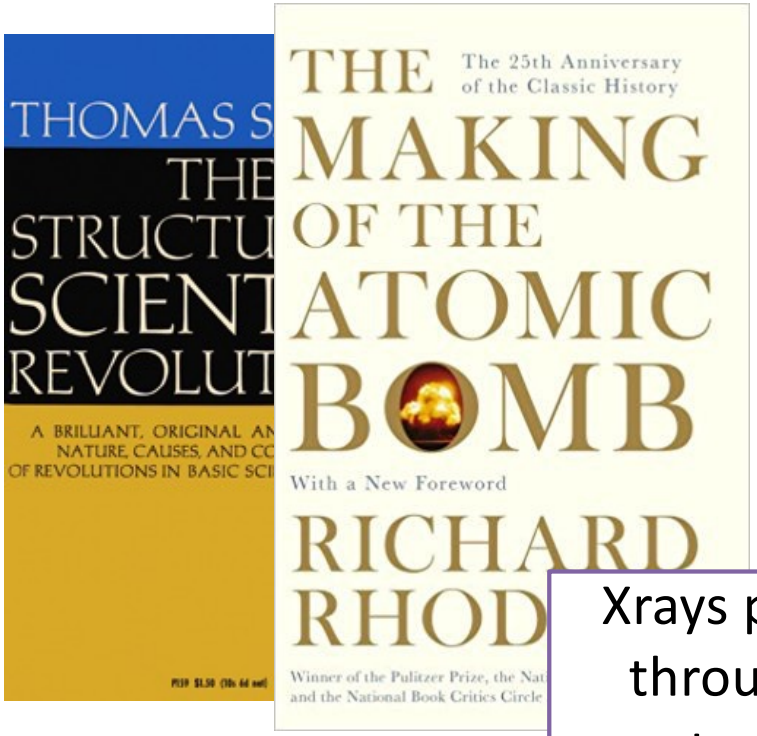
"… [S] scientific integrity, a principle of scientific thought that corresponds to a kind of utter honesty. You must do the best you can—if you know anything at all wrong, or possibly wrong—to explain it.

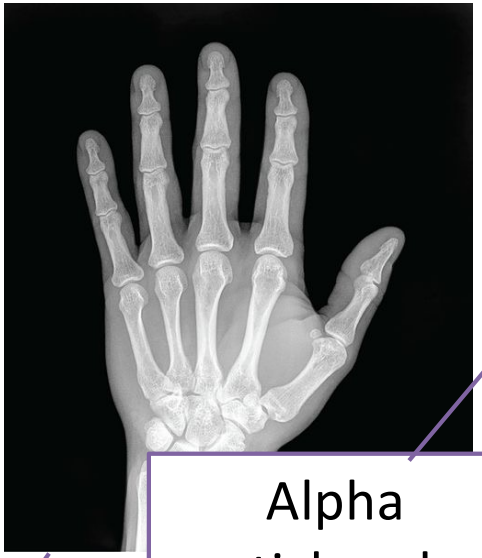
"Cargo Cult Science - Some remarks on science, pseudoscience, and learning how to not fool yourself. Caltech's 1974 commencement address. – Richard Feynman

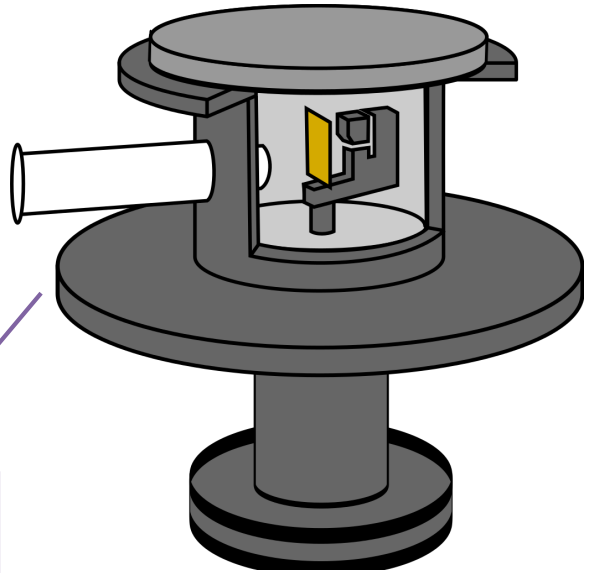
Editorial Comment

- The most exciting phrase to hear in science, the one that heralds new discoveries, is not “Eureka!” (I found it) but “That’s funny”
  - Attributed to Isaac Asimov (and others)

Editorial Comment

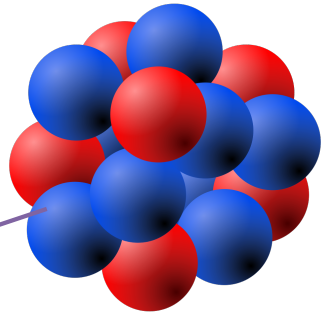






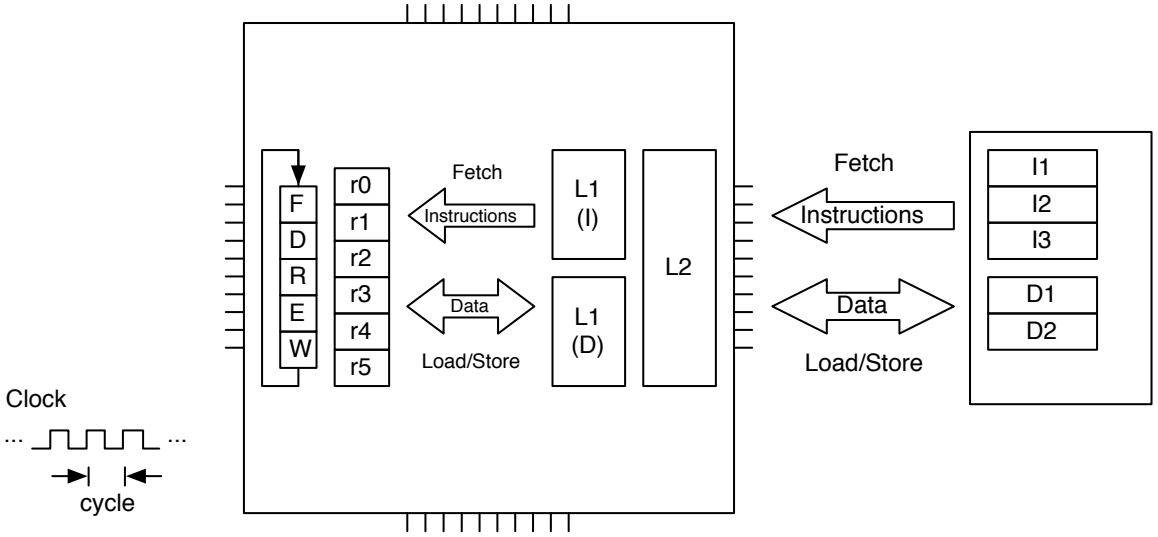
Xrays pass through materials

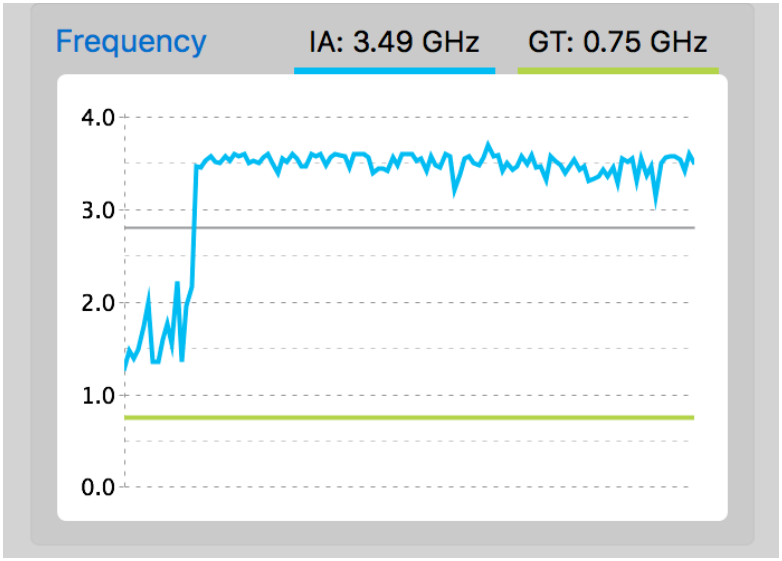
Alpha particles also, except small bit of noise



Which turned out to be the nucleus

Peak Performance vs Achieved Performance



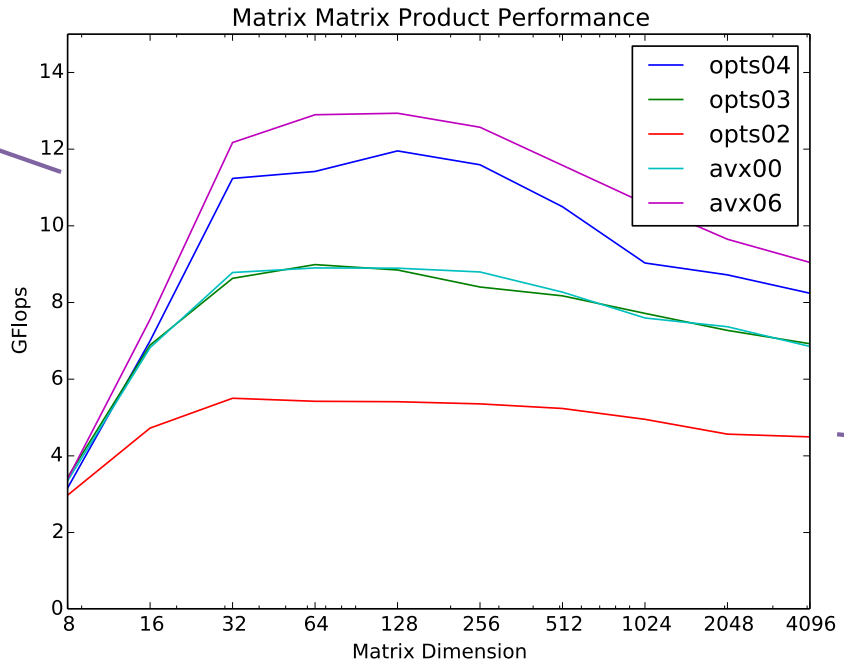


$$5 \times 10^9 \frac{\text{FLOPS}}{\text{second}} \div 3.5 \times 10^9 \frac{\text{cycles}}{\text{second}} \approx 1.5 \frac{\text{FLOPS}}{\text{cycle}}$$

That's funny

Even Funnier

What magic got these?



Former best performance

$$13 \times 10^9 \frac{\text{FLOPS}}{\text{second}} \div 3.5 \times 10^9 \frac{\text{cycles}}{\text{second}} \approx 3.7 \frac{\text{FLOPS}}{\text{cycle}}$$

Writing Faster Matrix Matrix Product

```
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);
  }
}
```

Intel advanced vector extensions

(Intrinsics for)

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

Vector load

Vector multiply

Vector add

Writing Faster Matrix Matrix Product

```
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);
  }
}
```

256 bit #

Double is 8 bytes (64 bits)

256 bit load

Four doubles

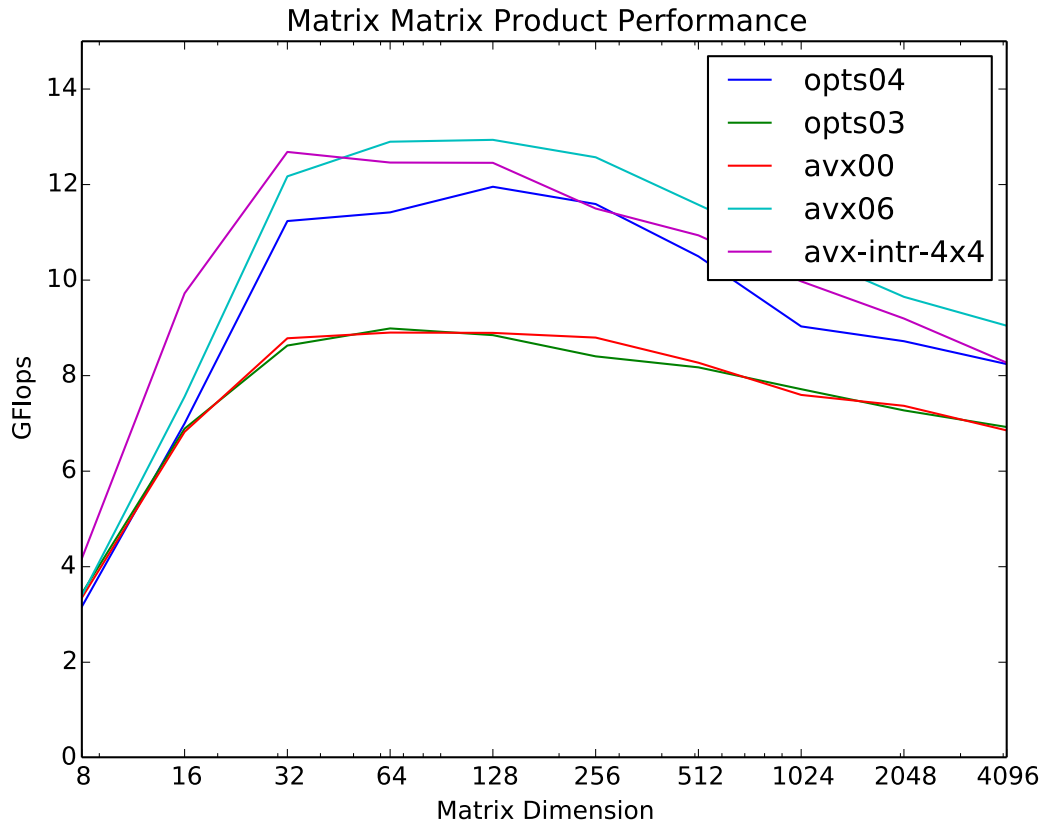
```
__m256d a0 = _mm256_broadcast_sd(&A(i  ,k));
a0  = _mm256_mul_pd(bx,  a0);
t0x = _mm256_add_pd(t0x, a0);
```

256 bit multiply (1 instruction)

256 bit add

Four FLOPS per cycle

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);
  }
}
```

X86 Assembly

AVX instructions

256 bit register

```
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
```

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;
  }
}
```

Fused Multiply-Add

256 bit registers

```
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
```

Compilation Process in More Detail (LLVM)

- LLVM (Low Level Virtual Machine) began as a research project at UIUC (Chris Lattner and Vikram Adve)
- Language independent infrastructure for building compilers
- Open source and widely used (supplanting gcc)
- Clang (C-language) front-end
- LLDB debugger

Ideal Compiler

Ideal Compiler

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) {
```

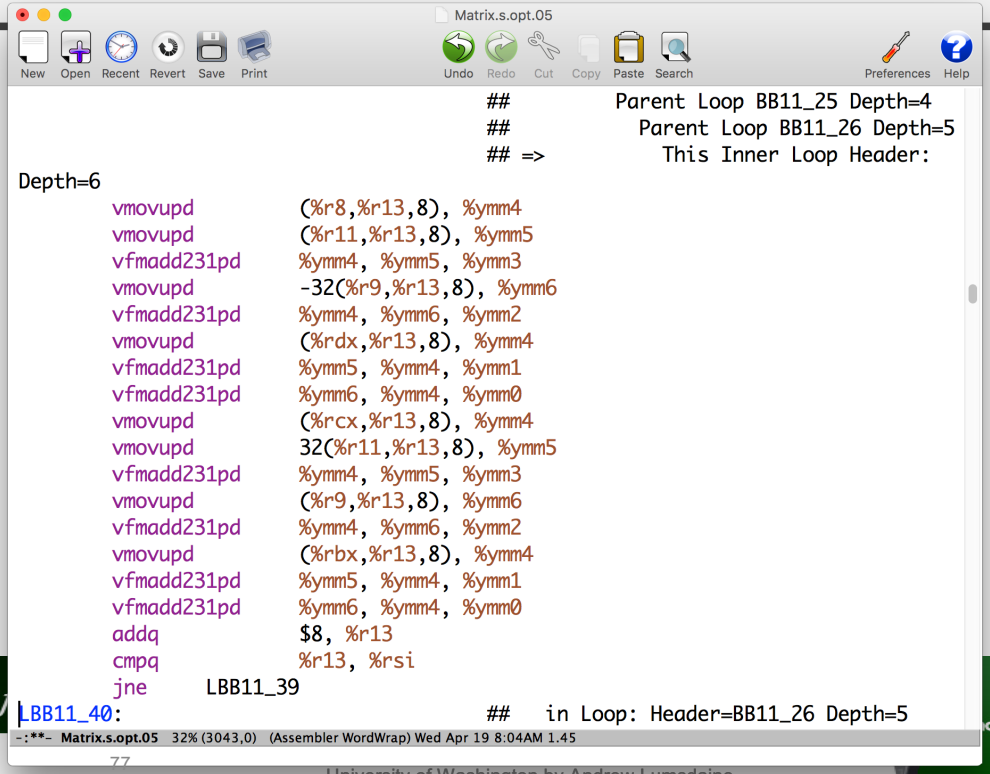
```
      for (int j = 0; j < B.numCols(); ++j) {
        double t = C(i,j);
        for (int k = 0; k < A.numCols(); ++k) {
          t += A(i,k) * B(k,j);
        }
        C(i,j) = t;
      }
```

Selects all

Unroll
Vectorization
Inline

As a Last Resort

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



Advanced Vector Extensions

SIMD?

Multi Media Extensions

Streaming SIMD Extensions

Advanced Vector Extensions

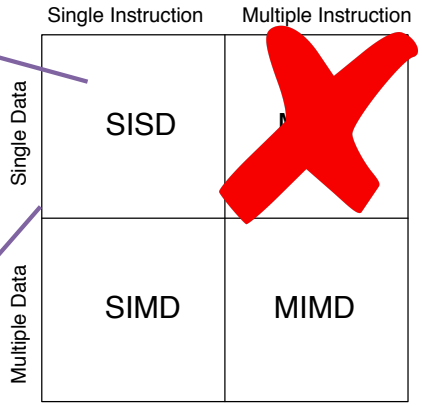
1980	1997	1999	2001	2004 2006 2007 2008	2011	2013	2016
8087	MMX	SSE	SSE2	SSE3 SSE3.1 SSE4.1 SSE4.2	AVX	AVX2	AVX512
							
8 80-bit stack registers	8 64-bit registers	8 128-bit registers (single) (xmm)	8 128-bit registers (double)	Many new instructions	16 256-bit registers (ymm)		32 512-bit registers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

Flynn's Taxonomy (Aside)

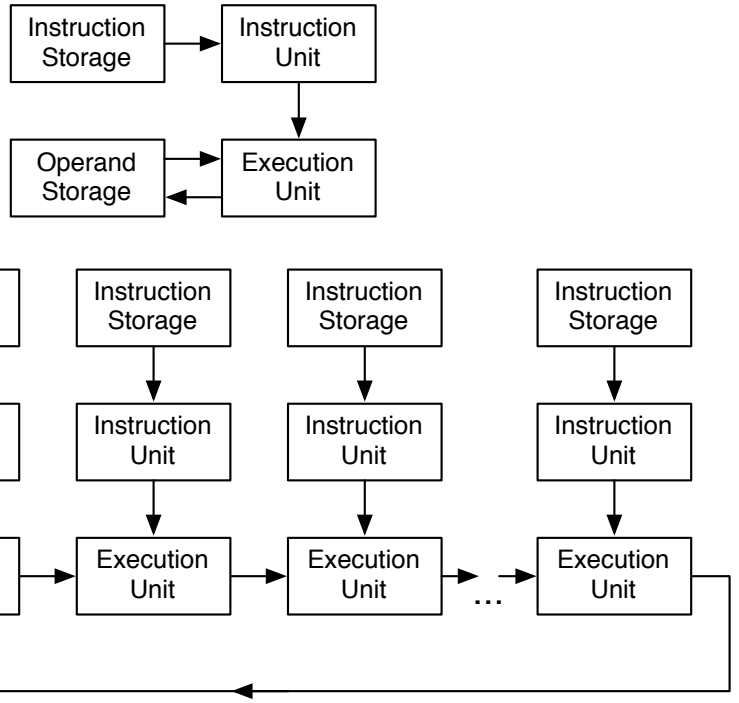
Anyone in HPC must know Flynn's taxonomy

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

Plain old sequential

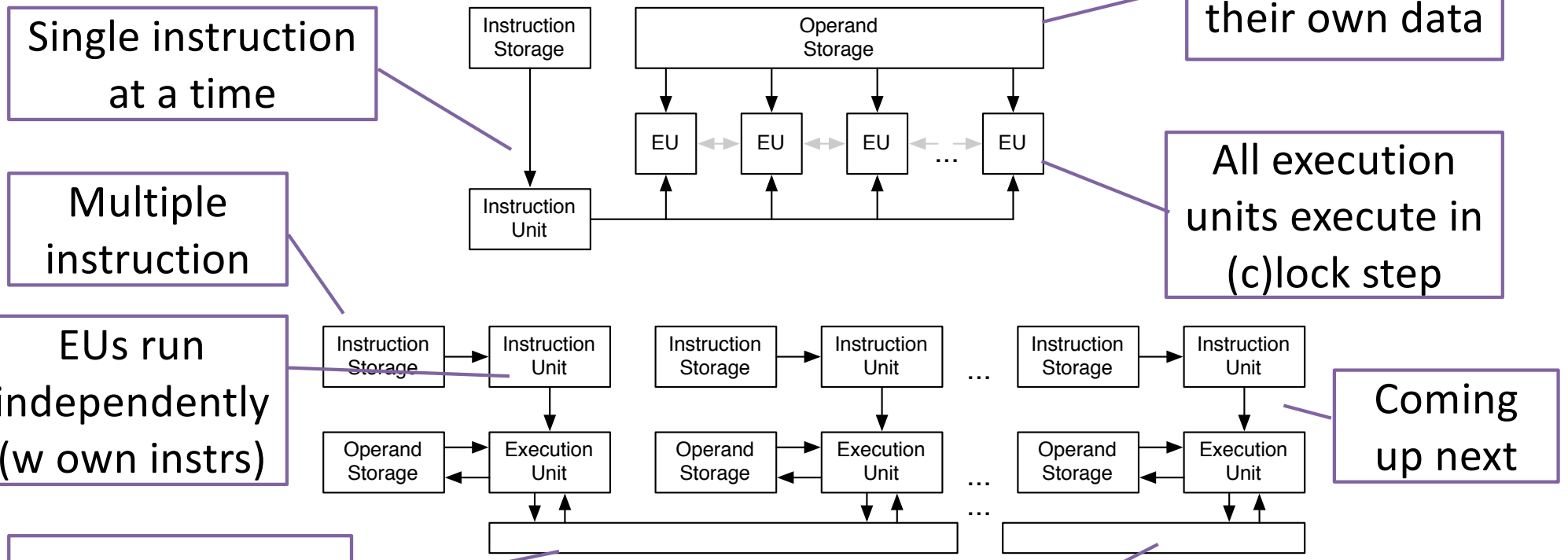


Based on multiplicity of instruction streams, data storage



SIMD and MIMD

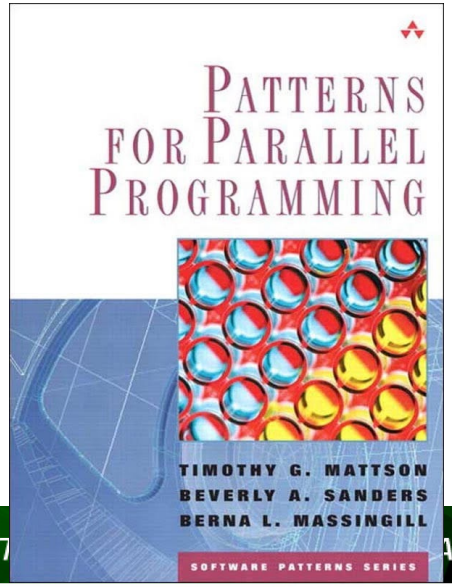
- Two principal parallel computing paradigms (multiple c

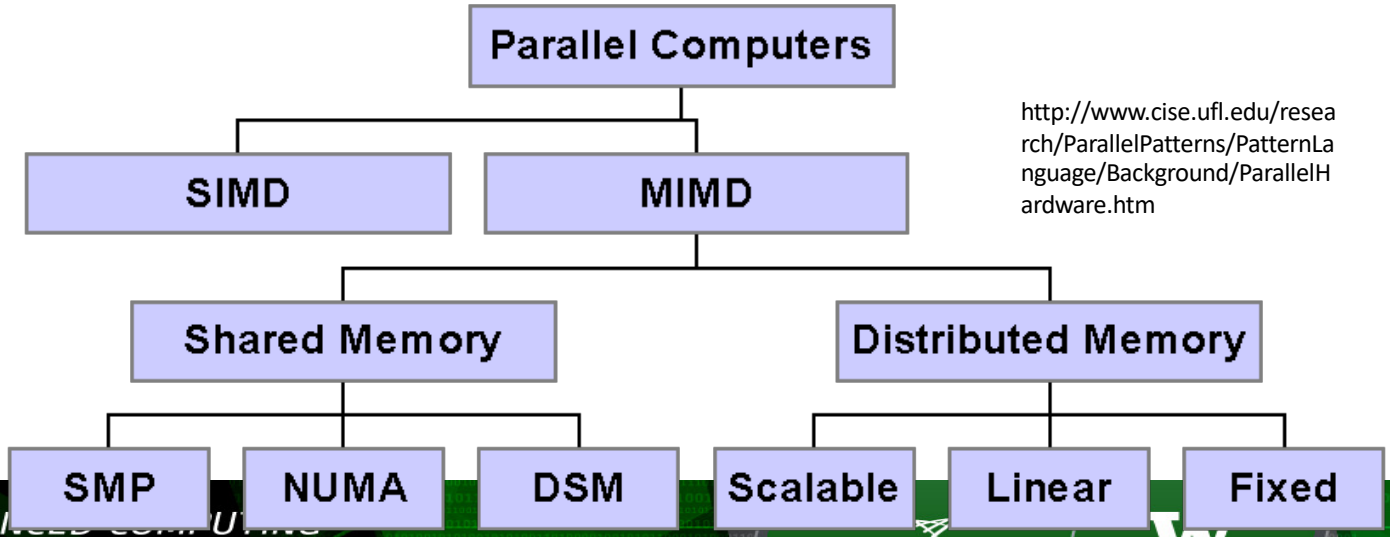


A More Refined (Programmer-Oriented) Taxonomy

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

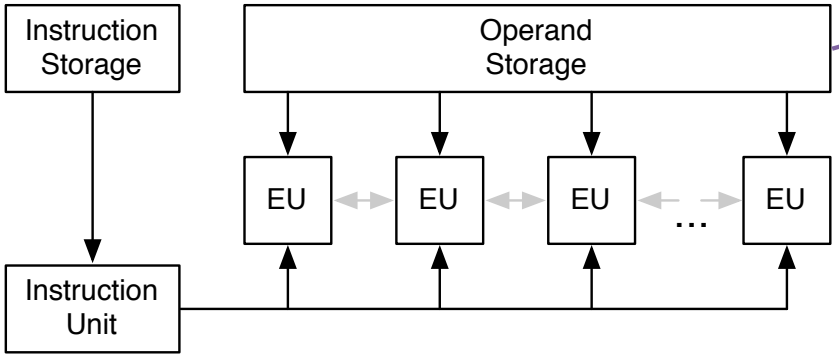
We will come back to this soon





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

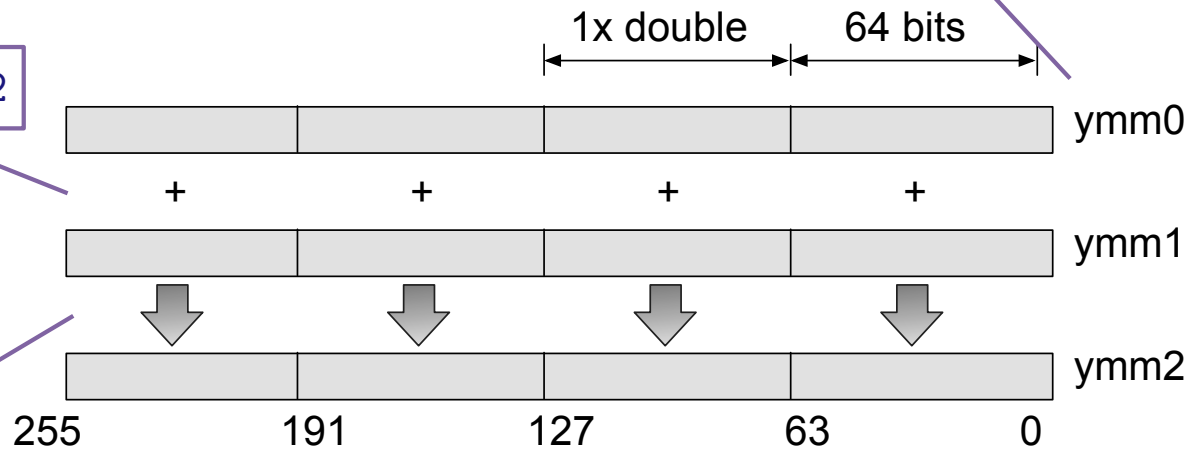
SIMD in SSE/AVX



Flynn's original conceptual model

ymm are 256 bit registers

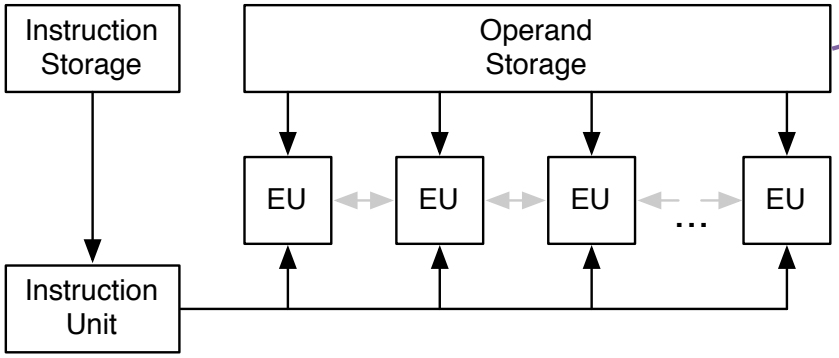
```
vfadd231pd  %ymm0, %ymm1, %ymm2
```



One machine instruction

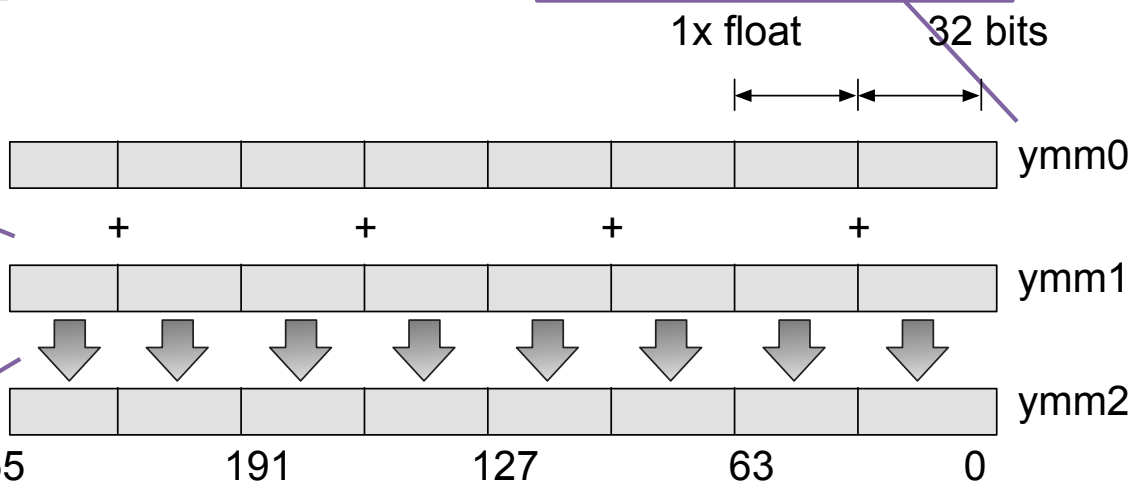
Adds all four doubles ***simultaneously***

SIMD in SSE/AVX



Flynn's original conceptual model

ymm are 256 bit registers

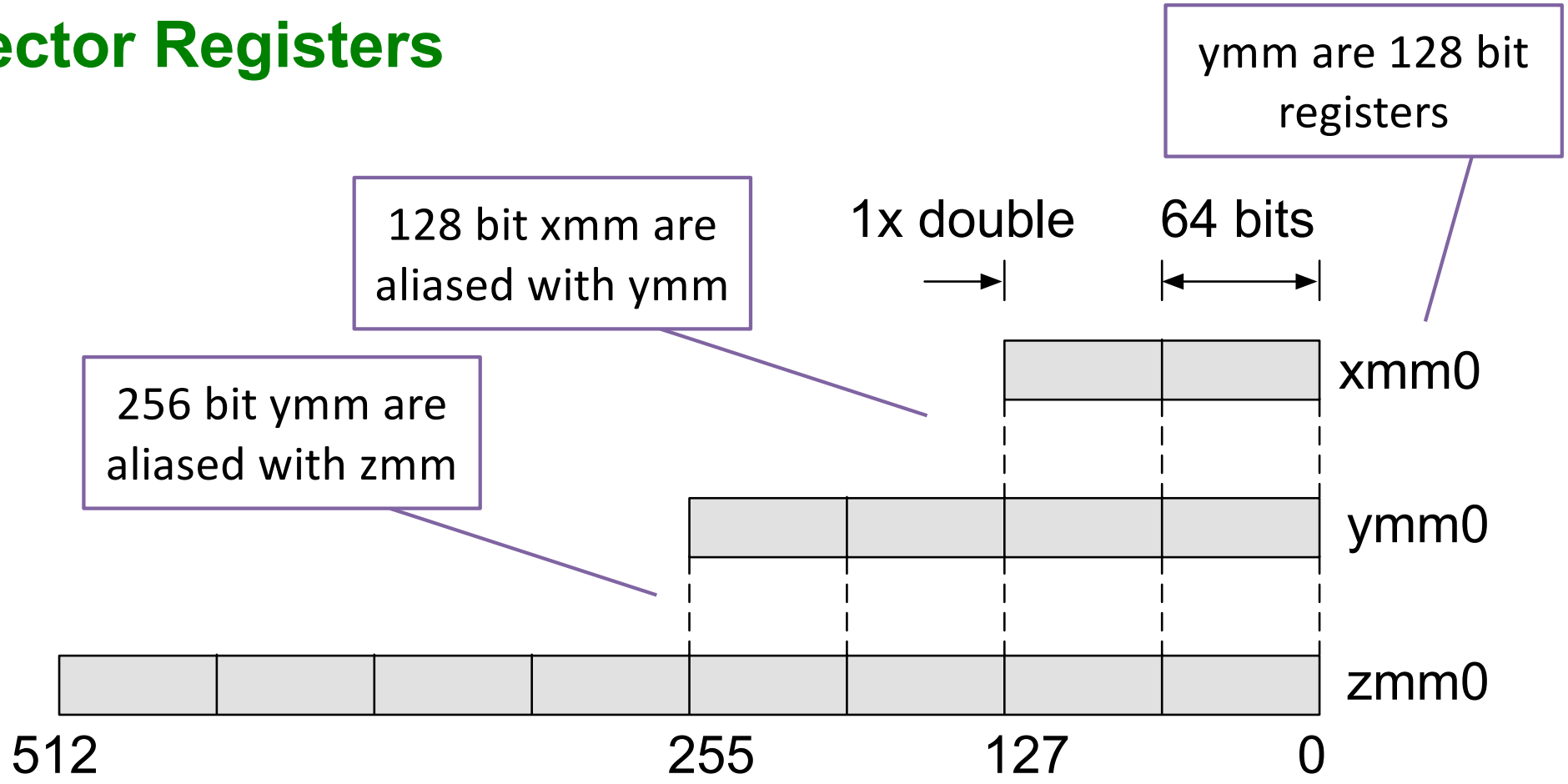



```
vfadd231ps  %ymm0, %ymm1, %ymm2
```

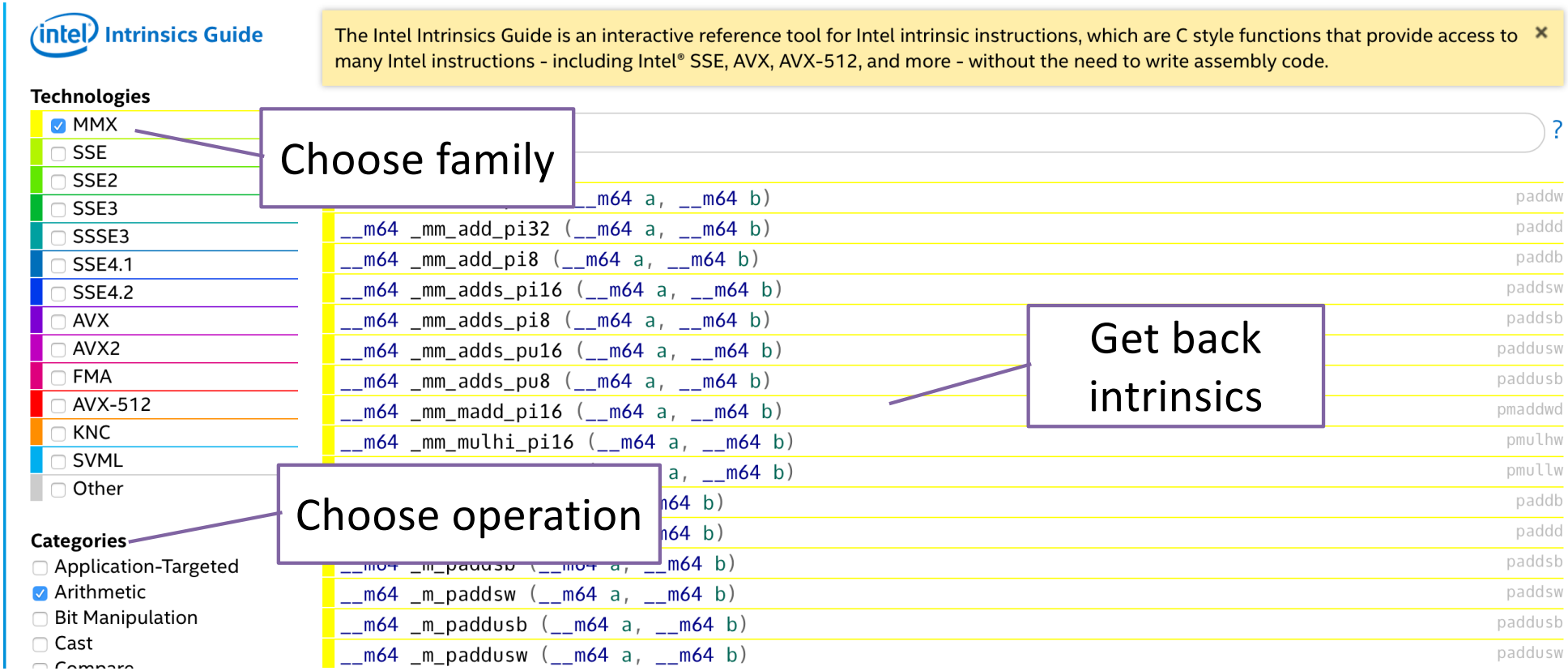
One machine instruction

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
```

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
```

Performance

Architecture	Latency	Throughput
Knights Landing	6	0.5

How to access AVX instructions from C/C++

The machine instruction(s) that is/are generated

Does your CPU support this instruction?

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

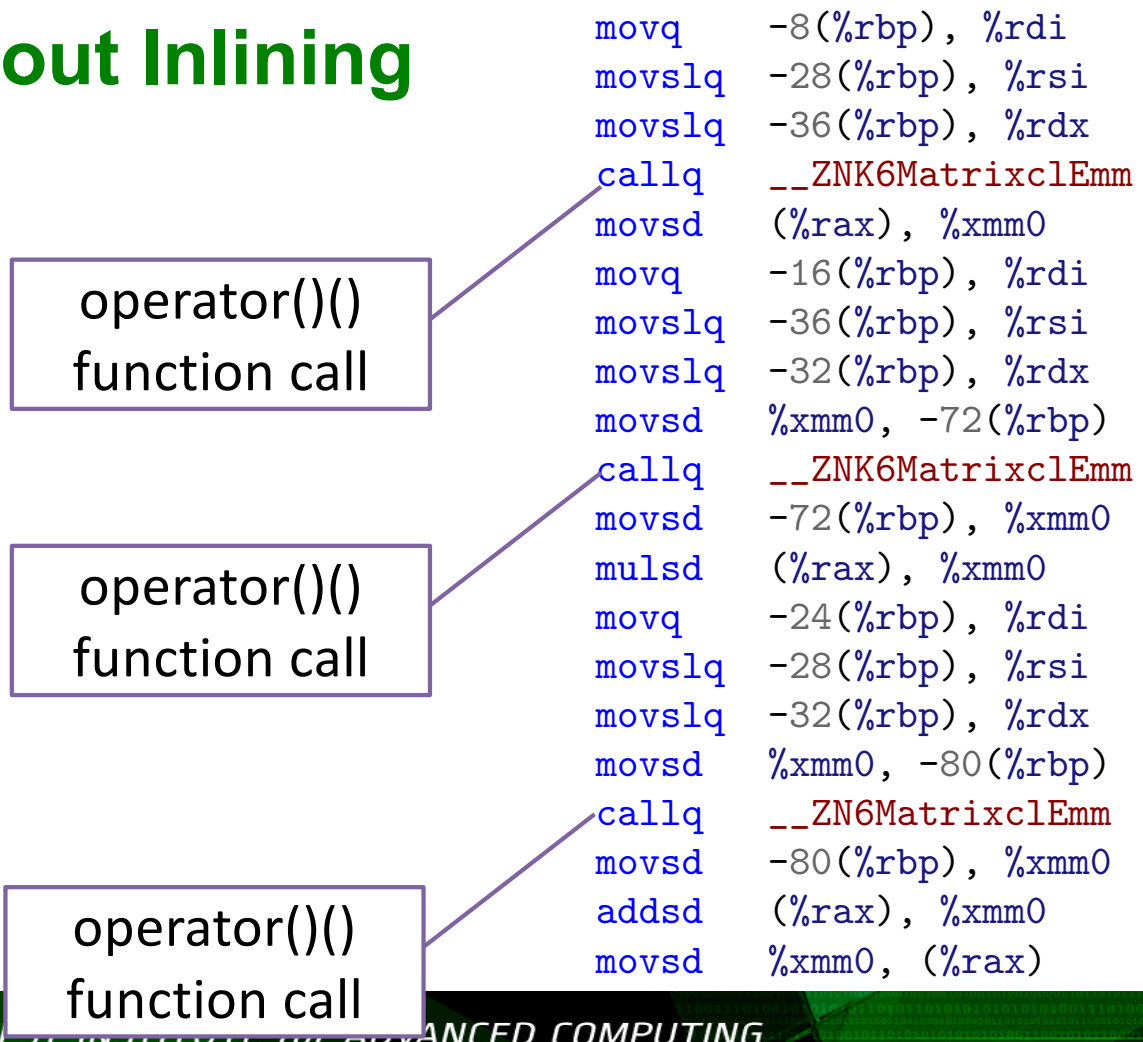
Easier if body is available to compiler

```
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!!

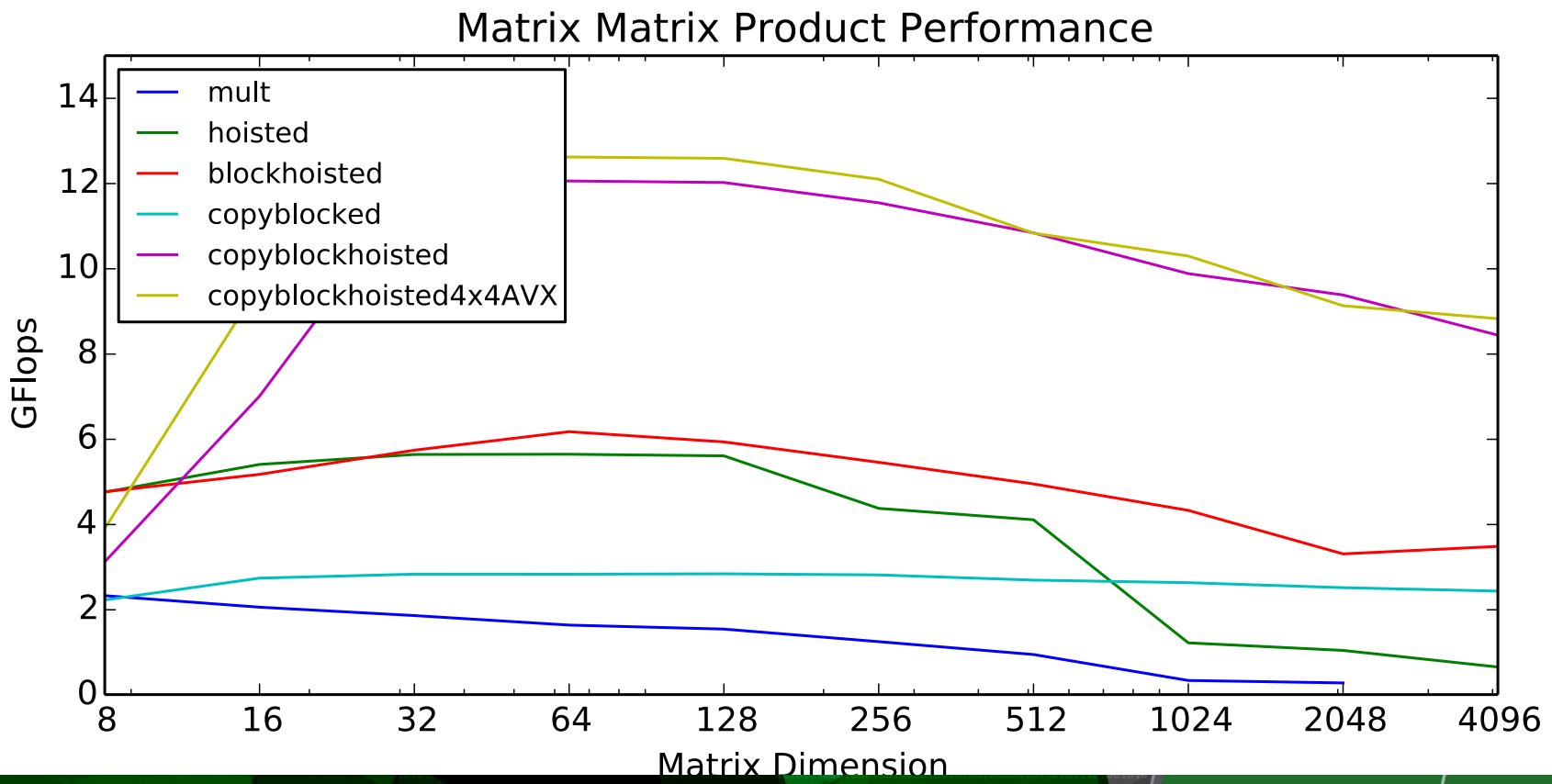
i.e., if it is ***defined in the header file***

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)
```

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

Tuning

How do we find the optimal combination?

Magic: the power of apparently influencing the course of events by using mysterious or supernatural forces

- Starting with base code
- Various compiler optimizations help
- Tiling (which size)
- Blocking (what size)
- What size works best for Tiling and Blocking ***together?***

- What loop ordering? Matrix matrix product has six different orderings? What block ordering?

- What about when we add AVX, and threads, etc?

The answer will be different for different CPUs

Finding the Sweet Spot

- Exhaustive parameter space search
  - Tiling, Blocking, Compiler flags, AVX inst, loop ordering
- Original project at UC Berkeley phiPAC (Bilmes et al)
- Further developed by Whaley and Dongarra → Automatically Tuned Linear Algebra Subprograms (ATLAS)
  - Recently honored with "test of time" award

And wrote a program to generate different multiply functions

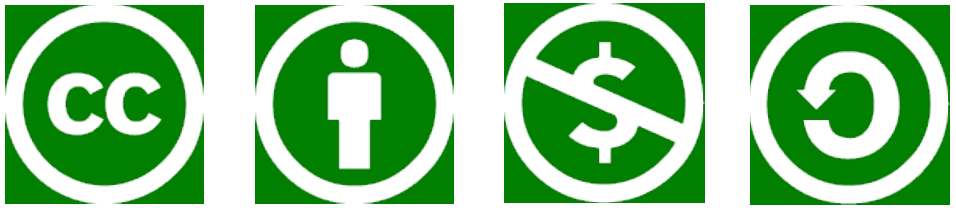
This started as a final course project

The competition was to write fastest matrix-matrix product

Students were the good kind of lazy

Thank You!

Creative Commons BY-NC-SA 4.0 License



© Andrew Lumsdaine, 2017-2018

Except where otherwise noted, this work is licensed under

https://creativecommons.org/licenses/by-nc-sa/4.0/