Lecture 2:
Tiling matrix-matrix multiply, code tuning

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Logistics

- Lecture notes and slides for first two lectures are up: `http://www.cs.cornell.edu/~bindel/class/cs5220-s10`.
- You should receive cluster information soon for `crocus.csuglab.cornell.edu`. When you do, make sure you can log in!
- We will be setting up a wiki for the class — among other things, this will be a way to form groups.
- Hope to have the first assignment ready by Wednesday.

Reminder: Matrix multiply

Consider naive square matrix multiplication:

```
#define A(i,j) AA[j*n+i]
#define B(i,j) BB[j*n+i]
#define C(i,j) CC[j*n+i]

for (i = 0; i < n; ++i) {
  for (j = 0; j < n; ++j) {
    C(i,j) = 0;
    for (k = 0; k < n; ++k)
      C(i,j) += A(i,k)*B(k,j);
  }
}
```

How fast can this run?

Why matrix multiply?

- Key building block for dense linear algebra
- Same pattern as other algorithms (e.g. transitive closure via Floyd-Warshall)
- Good model problem (well studied, illustrates ideas)
- Easy to find good libraries that are hard to beat!

1000-by-1000 matrix multiply on my laptop

- Theoretical peak: 10 Gflop/s using both cores
- Naive code: 330 MFlops (3.3% peak)
- Vendor library: 7 Gflop/s (70% peak)

Tuned code is $20\times$ faster than naive!

Simple model

Consider two types of memory (fast and slow) over which we have complete control.

- m = words read from slow memory
- t_m = slow memory op time
- f = number of flops
- t_f = time per flop
- $q = f/m$ = average flops / slow memory access

Time:

$$ft_f + mt_m = ft_f \left(1 + \frac{t_m/t_f}{q}\right)$$

Two important ratios:

- t_m/t_f = machine balance (smaller is better)
- q = computational intensity (larger is better)

How big can q be?

1. Dot product: n data, $2n$ flops
2. Matrix-vector multiply: n^2 data, $2n^2$ flops
3. Matrix-matrix multiply: $2n^2$ data, $2n^2$ flops

These are examples of level 1, 2, and 3 routines in *Basic Linear Algebra Subroutines* (BLAS). We like building things on level 3 BLAS routines.

q for naive matrix multiply

$q \approx 2$ (on board)

Better locality through blocking

Basic idea: rearrange for smaller working set.

```
for (I = 0; I < n; I += bs) {
  for (J = 0; J < n; J += bs) {
    block_clear(&(C(I,J)), bs, n);
    for (K = 0; K < n; K += bs)
      block_mul(&(C(I,J)), &(A(I,K)), &(B(K,J)),
                bs, n);
  }
}
```

Q: What do we do with “fringe” blocks?

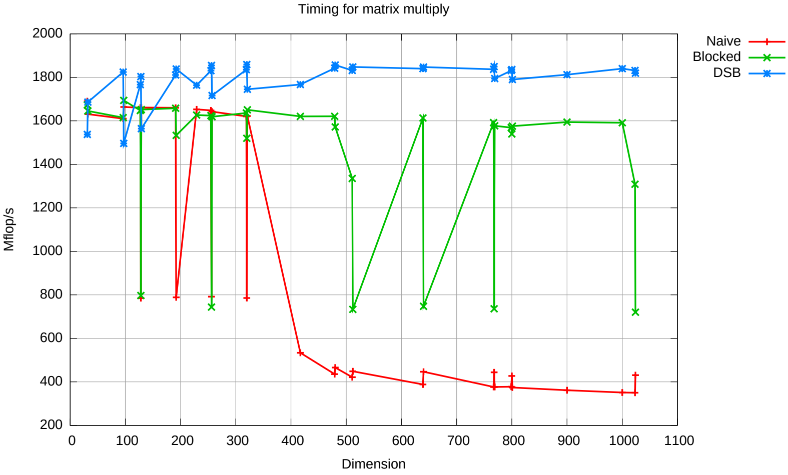
q for naive matrix multiply

$q \approx b$ (on board). If M_f words of fast memory, $b \approx \sqrt{M_f/3}$.

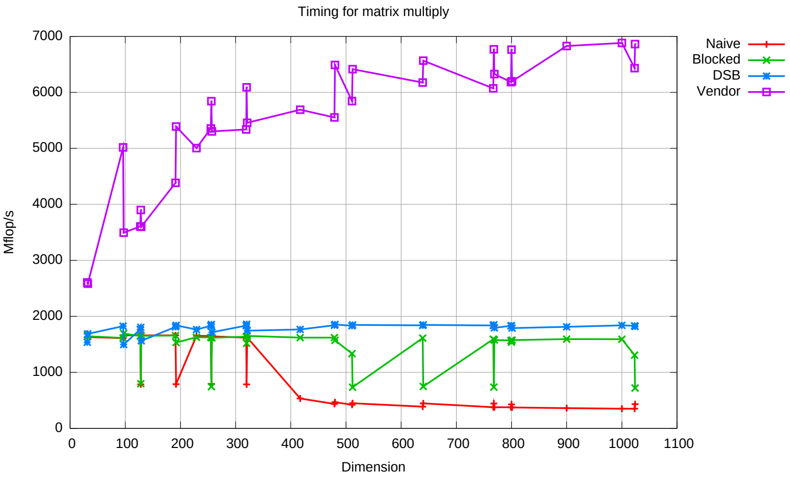
Th: (Hong/Kung 1984, Irony/Tishkin/Toledo 2004): Any reorganization of this algorithm that uses only associativity and commutativity of addition is limited to $q = O(\sqrt{M_f})$

Note: Strassen uses distributivity...

Better locality through blocking



Truth in advertising



Recursive blocking

- Can use blocking idea recursively (for L2, L1, registers)
- Best blocking is *not* obvious!
- Need to tune bottom level carefully...

Idea: Cache-oblivious algorithms

Index via Z-Morton ordering (“space-filling curve”)

- Pro: Works well for any cache size
- Con: Expensive index calculations

Good idea for ordering meshes?

Copy optimization

Copy blocks into contiguous memory

- Get alignment for SSE instructions (if applicable)
- Unit stride even across bottom
- Avoid *conflict* cache misses

Auto-tuning

Several different parameters:

- Loop orders
- Block sizes (across multiple levels)
- Compiler flags?

Use automated search!

Idea behind ATLAS (and earlier efforts like PhiPAC).

My last matrix multiply

- Good compiler (Intel C compiler) with hints involving aliasing, loop unrolling, and target architecture. Compiler does auto-vectorization.
- L1 cache blocking
- Copy optimization to aligned memory
- Small ($8 \times 8 \times 8$) matrix-matrix multiply kernel found by automated search. Looped over various size parameters.

On that machine, I got 82% peak. Here... less than 50% so far.

Tips on tuning

> *"We should forget bout small efficiences, say about 97% of the time: premature optimization is the root of all evil."*
> *– C.A.R. Hoare (quoted by Donald Knuth)*

- Best case: good algorithm, efficient design, *obvious code*
- Tradeoff: speed vs readability, debuggability, maintainability...
- Only optimize when needful
- Go for low-hanging fruit first: data layouts, libraries, compiler flags
- Concentrate on the bottleneck
- Concentrate on inner loops
- Get correctness (and a test framework) first

Tuning tip 0: use good tools

- We have `gcc`. The Intel compilers are better.
- Fortran compilers often do better than C compilers (less aliasing)
- Intel VTune, cachegrind, and Shark can provide useful profiling information (including information about cache misses)

Tuning tip 1: use libraries!

- Tuning is painful! You will see...
- Best to build on someone else's efforts when possible

Tuning tip 2: compiler flags

- `-O3`: Aggressive optimization
- `-march=core2`: Tune for specific architecture
- `-ftree-vectorize`: Automatic use of SSE (supposedly)
- `-funroll-loops`: Loop unrolling
- `-ffast-math`: Unsafe floating point optimizations

Sometimes *profiler-directed* optimization helps. Look at the gcc man page for more.

Tuning tip 3: Attend to memory layout

- Arrange data for unit stride access
- Arrange algorithm for unit stride access!
- Tile for multiple levels of cache
- Tile for registers (loop unrolling + “register” variables)

Tuning tip 4: Use small data structures

- Smaller data types are faster
  - Bit arrays vs int arrays for flags?
  - Minimize indexing data — store data in blocks
  - Some advantages to *mixed precision* calculation (`float` for large data structure, `double` for local calculation) — more later in the semester!
- Sometimes recomputing is faster than saving!

Tuning tip 5: Inline judiciously

- Function call overhead *often* minor...
- ... but structure matters to optimizer!
- C++ has `inline` keyword to indicate inlined functions

Tuning tip 6: Avoid false dependencies

Arrays in C can be aliased:

```
a[i]   = b[i] + c;
a[i+1] = b[i+1] * d;
```

Can't reorder – what if `a[i+1]` refers to `b[i]`? But:

```
float b1 = b[i];
float b2 = b[i+1];
a[i]   = b1 + c;
a[i+1] = b2 * d;
```

Declare no aliasing via restrict pointers, compiler flags, pragmas...

Tuning tip 7: Beware inner loop branches!

- Branches slow down code if hard to predict
- May confuse optimizer that only deals with basic blocks

Tuning tip 8: Preload into local variables

```
while (...) {
  *res++ = filter[0]*signal[0] +
           filter[1]*signal[1] +
           filter[2]*signal[2];
  signal++;
}
```

Tuning tip 8: Preload into local variables

... becomes

```
float f0 = filter[0];
float f1 = filter[1];
float f2 = filter[2];
while (...) {
  *res++ = f0*signal[0] +
           f1*signal[1] +
           f2*signal[2];
  signal++;
}
```

Tuning tip 9: Loop unrolling plus software pipelining

```
float s0 = signal[0], s1 = signal[1],
      s2 = signal[2];
*res++ = f0*s0 + f1*s1 + f2*s2;
while (...) {
  signal += 3;
  s0 = signal[0];
  res[0] = f0*s1 + f1*s2 + f2*s0;
  s1 = signal[1];
  res[1] = f0*s2 + f1*s0 + f2*s1;
  s2 = signal[2];
  res[2] = f0*s0 + f1*s1 + f2*s2;
  res += 3;
}
```

Note: more than just removing index overhead!
Remember: `-funroll-loops`!

Tuning tip 10: Expose independent operations

- Use local variables to expose independent computations
- Balance instruction mix for different functional units

```
f1 = f5 * f9;
f2 = f6 + f10;
f3 = f7 * f11;
f4 = f8 + f12;
```

Examples

What to use for high performance?

- Function calculation or table of precomputed values?
- Several (independent) passes over a data structure or one combined pass?
- Parallel arrays vs array of records?
- Dense matrix vs sparse matrix (only nonzeros indexed)?
- MATLAB vs C for dense linear algebra codes?

Your assignment (out Weds)

- Learn to log into cluster.
- Find someone to work with (wiki should help? assigned?)
- Optimize square matrix-matrix multiply.

Details and pointers to resources in next couple days.