Session 5: Cache blocking/tiling

COMP52315: performance engineering

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An exemplar problem

Matrix transpose

$$B_{ij} \leftarrow A_{ji} \quad A, B \in \mathbb{R}^{n \times n}$$

```c
double *a, *b;
...
for (int i = 0; i < N; i++)
  for (int j = 0; j < N; j++)
    b[i*N + j] = a[j*N + i];
```

So far, we've talked about how to measure performance, and perhaps determine that it is bad.

$\Rightarrow$ what can we do about it?

Matrix transpose: simple performance model

Set up our expectation

- N^2 loads, N^2 stores, no compute

$\Rightarrow$ all we're doing is copying data

- Hence we might expect to see performance close to that of the streaming memory bandwidth, independent of matrix size.

Matrix transpose: simple performance model

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- Hence we might expect to see performance close to that of the streaming memory bandwidth, independent of matrix size.

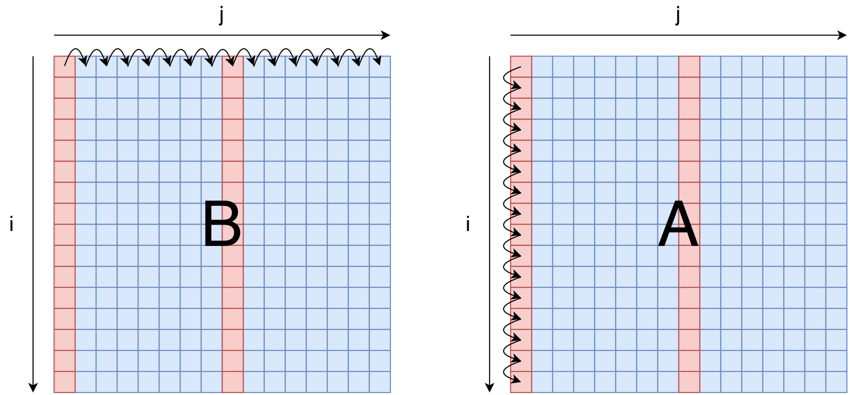
Matrix size	BW [GByte/s]
128×128	22
256×256	13
512×512	13
1024×1024	5
2048×2048	1.6
4096×4096	0.9

What went wrong?

```c
double *a, *b;
...
for (int i = 0; i < N; i++)
  for (int j = 0; j < N; j++)
    b[i*N + j] = a[j*N + i];
```

- We have streaming access to `b`, but stride-N access to `a`.
- If both matrices fit in cache, this is OK, and a reasonable model of time is $T_{\text{cache}} = N^2(t_{\text{read}} + t_{\text{write}})$.
- Note that the reads of `a` load a full cache line, but use only 8 bytes of it.
- Better model $T_{\text{mem}} = N^2(8t_{\text{read}} + t_{\text{write}})$

A picture



Cache locality

- Since we have strided access to `a`, we need to hold LN bytes in the cache to get any reuse, where L is the cache line size in. This is not possible for large matrices.
- A mechanism to fix this is to *reorder* the loop iterations to preserve spatial locality.

Idea

- Break loop iteration space into blocks
    - *strip-mining*
    - *loop reordering*

Strip mining

- Break a loop into blocks of consecutive elements

Before

```
for ( int i = 0; i < N; i++ )
  a[i] = f(i);
```

After

```
for ( int ii = 0; ii < N; ii += stride)
  for ( int i = ii; i < min(N, ii + stride); i++)
    a[i] = f(i);
```

- Not that useful for just a single loop, although there are circumstances where one might use it

Strip mining multiple loops

- Let’s do the same for both loops of the transpose:

Before

```
for (int i = 0; i < N; i++)
  for (int j = 0; j < N; j++)
    a[i*N + j] = a[j*N + i];
```

After

```
for (int ii = 0; ii < N; ii += stridei)
  for (int i = ii; i < min(N, ii+stridei); i++)
    for (int jj = 0; jj < N; jj += stridej)
      for (int j = jj; j < min(N, jj+stridej); j++)
        b[i*N + j] = a[j*N + i];
```

- Haven’t yet made any change to the performance

Reorder loops

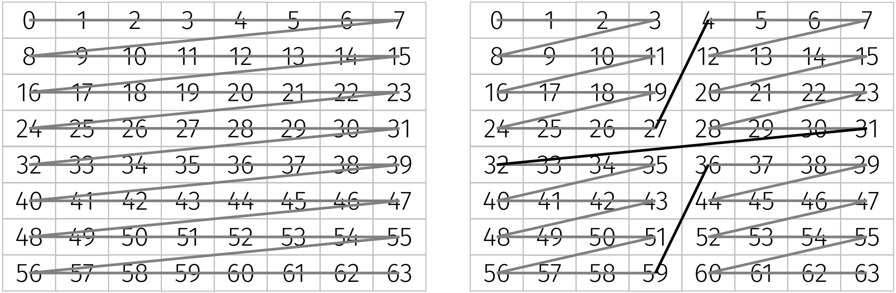
After permuting `i` and `jj` loops

```
for (int ii = 0; ii < N; ii += stridei)
  for (int jj = 0; jj < N; jj += stridej)
    for (int i = ii; i < min(N, ii+stridei); i++)
      for (int j = jj; j < min(N, jj+stridej); j++)
        b[i*N + j] = a[j*N + i];
```

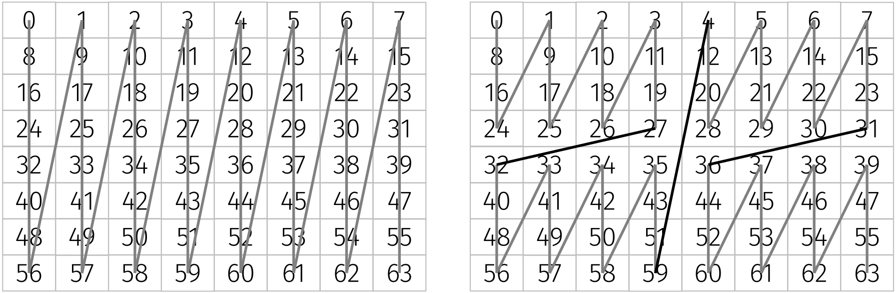
- Two free parameters `stridei` and `stridej`
- Need to choose these appropriately to levels in the cache hierarchy
- Ideally block for L1, L2, L3, etc…
- The extra logic adds some overhead

Why is it "tiling"?

Iteration over *B*.



Iteration over A.



Does it work?

- Have a go, I provide some sample code for which you can tune the blocking parameters.

$\Rightarrow$ Exercise 7.

A second problem

Matrix-Matrix multiplication

$$C_{ij} \leftarrow C_{ij} + \sum_k A_{ik} B_{kj} \quad A, B, C \in \mathbb{R}^{n \times n}$$

```c
for (int i = 0; i < n; i++)
  for (int j = 0; j < n; j++)
    for (int k = 0; k < n; k++)
      C[i*n + j] += A[i*n + k] * B[k*n + j];
```

Same story here (or at least it was in the 90s!).

(Another) simple model for computation

- Simple model of memory, two levels: "fast" and "slow"
- Initially all data in slow memory

m	number of data elements moved between fast and slow memory
t_m	time per slow memory operation
f	number of flops
$t_f \ll t_m$	time per flop
$q =: f/m$	average flops per slow memory access

- Minimum time to solution (all data in fast memory)

$$t_f f$$

- Typical time

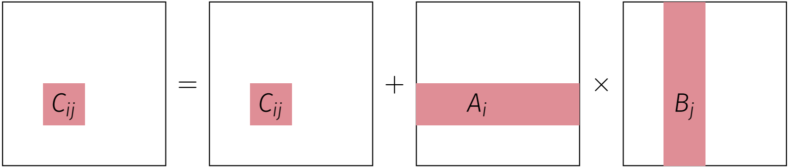
$$f t_f + m t_m = f t_f \left(1 + \frac{t_m}{t_f}\frac{1}{q}\right)$$

- t_m/t_f property of hardware, q property of *algorithm*

Naïve matrix-multiply

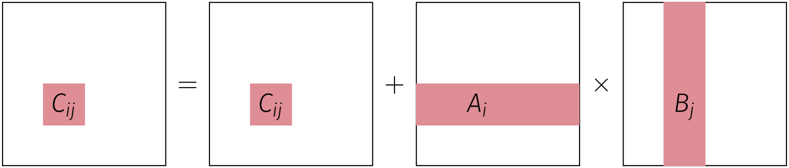
```c
for (int i = 0; i < n; i++)
  for (int j = 0; j < n; j++)
    for (int k = 0; k < n; k++)
      C[i*n + j] = C[i*n + j] + A[i*n + k] * B[k*n + j];
```

- Algorithm does $2n^3 = \mathcal{O}(n^3)$ flops and touches $3 \cdot 8n^2$ bytes of memory
- q potentially $\mathcal{O}(n)$, arbitrarily large for large n.



Naïve matrix-multiply

```
for (int i = 0; i < n; i++)
  // Read row i of A into fast memory
  for (int j = 0; j < n; j++)
    // Read C_ij into fast memory
    // Read column j of B into fast memory
    for (int k = 0; k < n; k++)
      C[i*n + j] = C[i*n + j] + A[i*n + k] * B[k*n + j];
    // Write C_ij back to slow memory
```



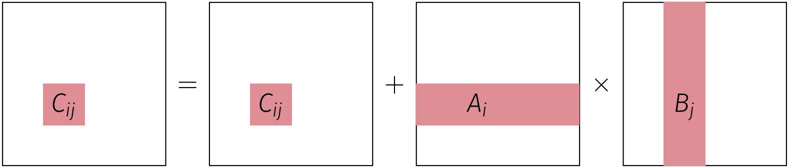
Naïve matrix-multiply

Number of slow memory references

$$
\begin{aligned}
m = n^3 &\quad \text{each column of } B \text{ is read } n \text{ times} \\
+ n^2 &\quad \text{each row of } A \text{ is read } n \text{ once} \\
+ 2n^2 &\quad \text{each entry of } C \text{ is read once and written once} \\
= (n^3 + 3n^2)
\end{aligned}
$$

Hence

$$\lim_{n\to\infty} q = \frac{f}{m} = \frac{2n^3}{(n^3 + 3n^2)} = 2$$



From model to prediction

- So for a triply-nested loop structure, the *best* time to solution our model predicts is:
$$T = t_f f \left(1 + \frac{t_m}{2t_f}\right)$$
- Recall that on modern hardware, memory *latency* is around 200 cycles per cache line. So let's approximate $t_m \approx 200/8 = 25$, and say $t_f = 1$.

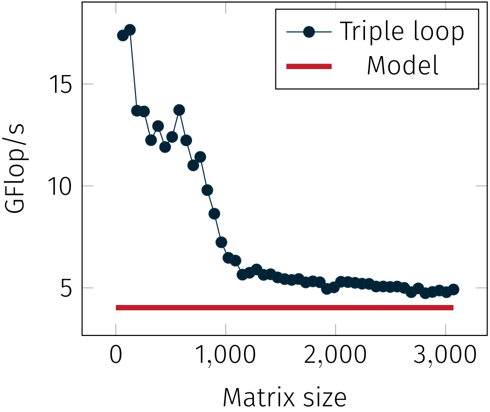
$$T = t_f f (1 + 25/2) = 13.5 t_f f$$

- Maximally 7% peak.
- This is *only* an estimate.

Measurement

- Single core Intel i5-8259U.
- 2 4-wide FMAs per cycle $\Rightarrow$ 16 DP FLOPs/cycle.

$\Rightarrow$ Peak is $3.6 \cdot 16 = 57.6$ GFLOPs/s, model predicts 4.03GFLOPs/s.



How to improve reuse?

- Problem is that we move rows and columns into fast memory, and then evict them
- Need way of keeping the loaded data in fast memory as long as possible.

$\Rightarrow$ tile iterations

```
// Treat A, B, C ∈ (ℝ^{b×b})^{N×N}
// that is, N × N matrices where each entry is a b × b matrix.
for (int i = 0; i < N; i++)
  for (int j = 0; j < N; j++)
    // Read block C_ij into fast memory
    for (int k = 0; k < n; k++)
      // Read block A_ik into fast memory
      // Read block B_kj into fast memory
      // Do matrix multiply on the blocks
      C[i*N + j] = C[i*N + j] + A[i*N + k] * B[k*N + j];
    // Write block C_ij back to slow memory
```

How to improve reuse?

- Problem is that we move rows and columns into fast memory, and then evict them
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$\Rightarrow$ tile iterations

```
// Treat A, B, C ∈ (ℝ^{b×b})^{N×N}
// that is, N × N matrices where each entry is a b × b matrix.
for (int ii = 0; ii < N; ii++)
  for (int jj = 0; jj < N; jj++)
    for (int kk = 0; kk < N; kk++)
      for (int i_ = 0; i_ < b; i_++)
        for (int j_ = 0; j_ < b; j_++)
          for (int k_ = 0; k_ < b; k_++) {
             const int i = ii*b + i_;
             const int j = jj*b + j_;
             const int k = kk*b + k_;
             C[i*n + j] = C[i*n + j] + A[i*n + k] * B[k*n + j];
          }
```

What did that do to the data movement?

$$
\begin{aligned}
m &= Nn^2 \quad \text{each block of } B \text{ is read } N^3 \text{ times} \Rightarrow N^3 b^2 = N^3 (n/N)^2 = Nn^2 \\
&+ Nn^2 \quad \text{each block of } A \text{ is read } N^3 \text{ times} \\
&+ 2n^2 \quad \text{each block of } C \text{ is read once and written once} \\
&= 2n^2(N+1)
\end{aligned}
$$

Hence

$$
\lim_{n\to\infty} q = \frac{f}{m} = \frac{2n^3}{2n^2(N+1)} = \frac{n}{N} = b
$$

- $b \gg 2$ so much better than previously. Can improve performance by increasing b *as long as blocks still fit in fast memory!*
- Detailed analysis of blocked algorithms in Lam, Rothberg, and Wolf *The Cache Performance and Optimization of Blocked Algorithms* (1991)

From model to machine characteristics

- Arbitrarily choose a “fast” algorithm to be $\geq 50\%$ peak, this requires

$$f t_f \left(1 + \frac{t_m}{t_f}\frac{1}{q}\right) \leq 2 t_f f \Leftrightarrow \frac{t_m}{t_f}\frac{1}{q} \leq 1 \Leftrightarrow q \geq \frac{t_m}{t_f}$$

- Again, approximate $t_m = 25$, $t_f = 1$

$\Rightarrow$ $b \approx q \geq 25$.

- Need to hold all three $b \times b$ matrices in cache

$\Rightarrow$ Need space for $3b^2 = 3 \cdot 25^2 = 1875$ matrix *entries*, approximately 14.6KB of fast memory M_{fast}.

- This is smaller than L1, but larger than fits in registers.

Is this the best we can do?

Theorem

Hong and Kung (1981) Any reorganization of this algorithm that only exploits associativity has

$$q = \mathcal{O}(\sqrt{M_{fast}})$$

and the number of data elements moved between slow and fast memory is

$$\Omega\left(\frac{n^3}{\sqrt{M_{fast}}}\right)$$

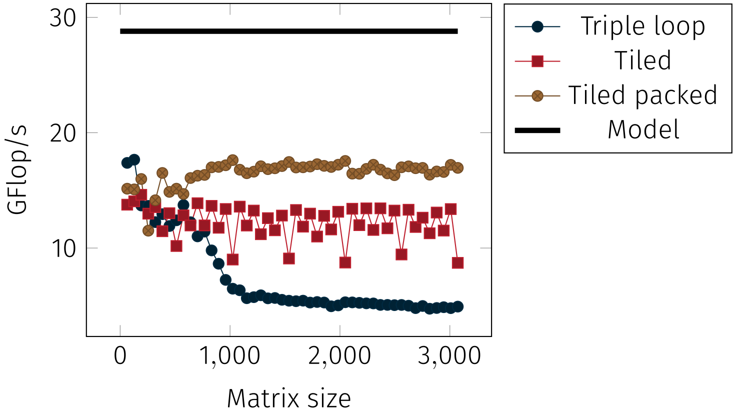
- Exact values for the bounds are not known, the best bounds are provided by Smith and van de Geijn (2017) `arXiv: 1702.02017 [cs.CC]`
- The GotoBLAS/OpenBLAS approach approaches these bounds.

Matching reality with models

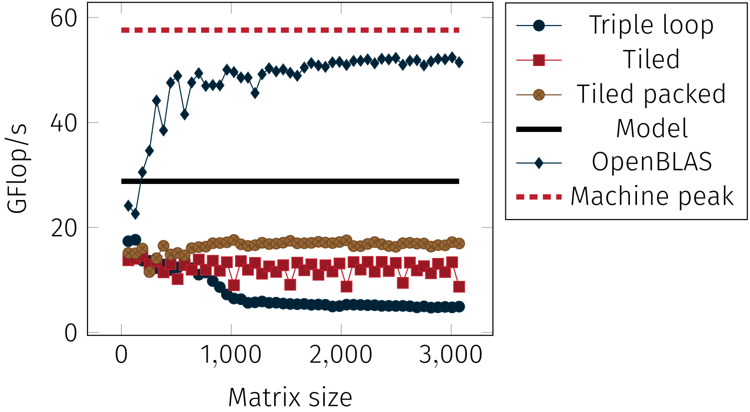
- I provide some sample code that implements this scheme

$\Rightarrow$ Exercise 8.

Is this the best we can do?



Is this the best we can do?



What accounts for this difference?

- Managed to get big matrices to behave like small ones with naive code.

$\Rightarrow$ reaching in-cache performance of the starting point.

- For better results, need to
  1. Block for registers and all levels of cache
  2. Perform data-layout transformation to promote (better) vectorisation
- Will look more at data layout transforms next time.

Summary

- Loop tiling can *significantly* improve performance of nested loops.
- Particularly important to exploit data reuse.
- For the “last mile” we have to do more. Mostly the same idea, but thinking hard about data layout and explicit vectorisation.
- Simple models can be used to motivate whether things are worth trying.