

Lecture 11: Continued optimizations on General Matrix-Matrix multiplication (GEMM)

Tuesday February 28th 2023

Logistics

- HW #2 due Friday
- You will get a practice midterm by end of week (not due, just for your own study)
- We'll go over the midterm next Tuesday

Today's lecture

- Flash review of GEMM theory from last lecture
- Additional optimizations: Blocking, transposition, cache line optimizations, etc.
- Some notes on correctness checking (essential for developing nontrivial optimizations)



GEMM: General-purpose Matrix-Matrix multiplication

Cornerstone of many numerical algorithms (including GPU-accelerated Deep Learning workloads)

Fast implementations available in MKL and other libraries

Great example for design of parallel optimizations (including both multi-threading and SIMD) as it's easy to prototype but trickier to optimize

Most clear example we've seen so far of a **compute-bound** kernel

Theory of GEMM operation

For simplicity: **A** and **B** are square NxN matrices

Each element of the matrix product C = A*B given as:

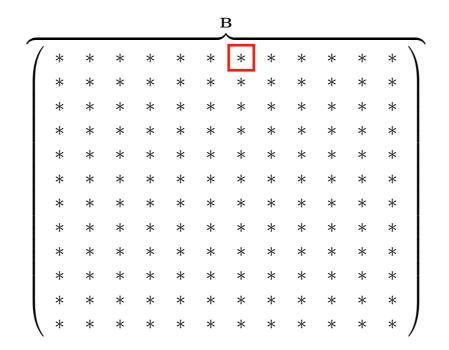
$$C_{ij} = \sum_{k=1}^{N} A_{ik} B_{kj}$$

In pseudocode:

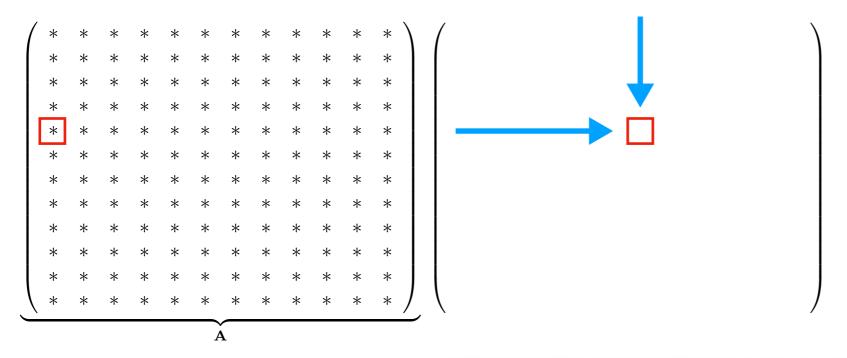
N^2 data and N^3 computation

$$ext{for } i = 1 \dots N$$
 $ext{for } j = 1 \dots N$ $ext{} C_{ij} \leftarrow 0$ $ext{for } k = 1 \dots N$ $ext{} C_{ij} \leftarrow C_{ij} + A_{ik} B_{kj}$

Theory of GEMM operation

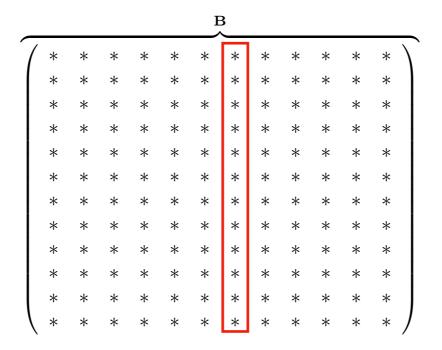


A visual illustration ...

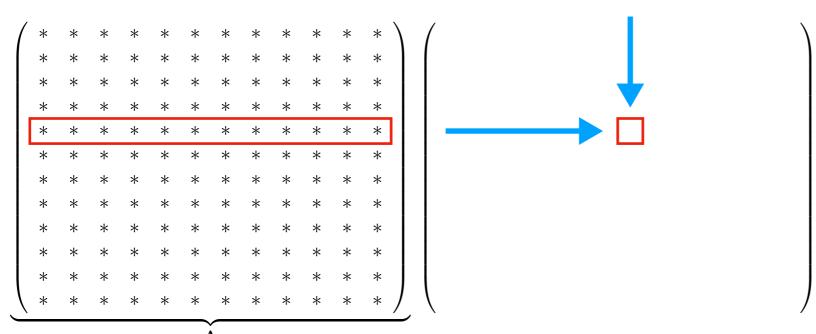


Multiply respective entries of **A** & **B**, accumulate on highlighted entry of **C=A*B**

Theory of GEMM operation



A visual illustration ...



$$\begin{array}{c} \texttt{for} \ i = 1 \dots N \\ \\ \texttt{for} \ j = 1 \dots N \\ \\ C_{ij} \leftarrow 0 \\ \\ \texttt{for} \ k = 1 \dots N \\ \\ C_{ij} \leftarrow C_{ij} + A_{ik}B_{kj} \end{array}$$

GEMM routine (MatMatMultiply.cpp)

|DenseAlgebra/GEMM_Test_0_0|

```
At matrix size = 1024
#include "MatMatMultiply.h"
void MatMatMultiply(const float (&A)[MATRIX_SIZE][MATRIX_SIZE],
    const float (&B)[MATRIX_SIZE][MATRIX_SIZE], float (&C)[MATRIX_SIZE][MATRIX_SIZE])
#pragma omp parallel for
    for (int i = 0; i < MATRIX_SIZE; i++)
   for (int j = 0; j < MATRIX_SIZE; j++) {
       C[i][j] = 0.;
                                                              Execution:
       for (int k = 0; k < MATRIX_SIZE;
                                        Running test iteration 1 [Elapsed time : 275.052ms]
           C[i][j] += A[i][k] * B[k][j];
                                          Running test iteration 2 [Elapsed time: 245.782ms]
                                          Running test iteration 3 [Elapsed time: 244.407ms]
                                          Running test iteration 4 [Elapsed time: 245.818ms]
                                          Running test iteration 5 [Elapsed time: 244.987ms]
                                          Running test iteration 6 [Elapsed time: 244.948ms]
                                          Running test iteration 7 [Elapsed time: 245.638ms]
                                          Running test iteration 8 [Elapsed time: 245.293ms]
                                          Running test iteration 9 [Elapsed time: 245.689ms]
                                          Running test iteration 10 [Elapsed time: 245.317ms]
```



GEMM routine (MatMatMultiply.cpp)

LDenseAlgebra/GEMM_Test_0_11

```
#include "MatMatMultiply.h"
#include "mkl.h"
void MatMatMultiply(const float (&A)[MATRIX_SIZE][MATRIX_SIZE],
    const float (&B)[MATRIX_SIZE][MATRIX_SIZE], float (&C)[MATRIX_SIZE][MATRIX_SIZE])
    cblas_sgemm(
        CblasRowMajor,
        CblasNoTrans,
        CblasNoTrans,
        MATRIX_SIZE,
        MATRIX_SIZE,
        MATRIX_SIZE,
        1.,
        &A[0][0],
        MATRIX_SIZE,
        &B[0][0],
        MATRIX_SIZE,
        0.,
        &C[0][0],
        MATRIX_SIZE
    );
```

We have replaced our hand-implemented code with a call to the BLAS **GEMM** routine



GEMM routine (MatMatMultiply.cpp)

LDenseAlgebra/GEMM_Test_0_11

```
#include "MatMatMultiply.h"
#include "mkl.h"
void MatMatMultiply(const float (&A)[MATRIX_SIZE][MATRIX_SIZE],
    const float (&B)[MATRIX_SIZE][MATRIX_SIZE], float (&C)[MATRIX_SIZE][MATRIX_SIZE])
    cblas_sgemm(
        CblasRowMajor,
        CblasNoTrans,
        CblasNoTrans,
        MATRIX_SIZE,
        MATRIX_SIZE,
        MATRIX_SIZE,
        1.,
                                                                Execution:
        A[0][0]
        MATRIX_SIZE,
        &B[0][0],
        MATRIX_SIZE,
        0.,
        &C[0][0],
       MATRIX_SIZE
```

At matrix size = 1024

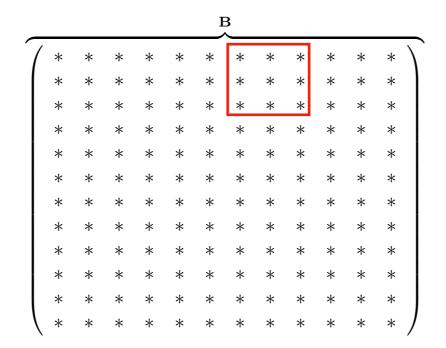
```
Running test iteration 1 [Elapsed time: 42.4088ms]
Running test iteration 2 [Elapsed time: 3.33403ms]
Running test iteration 3 [Elapsed time: 2.29802ms]
Running test iteration 4 [Elapsed time: 2.22505ms]
Running test iteration 5 [Elapsed time: 2.21731ms]
Running test iteration 6 [Elapsed time: 1.96854ms]
Running test iteration 7 [Elapsed time: 1.87623ms]
Running test iteration 8 [Elapsed time: 1.91837ms]
Running test iteration 9 [Elapsed time: 1.91348ms]
Running test iteration 10 [Elapsed time: 1.90199ms]
```

GEMM routine (MatMatMultiply.cpp)

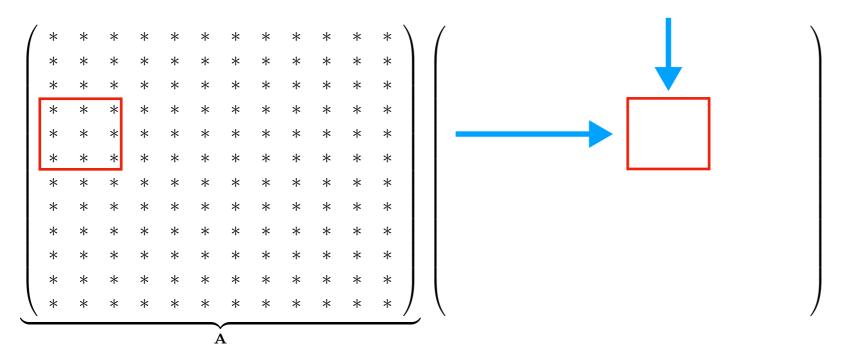
|DenseAlgebra/GEMM_Test_0_2|

```
#include "MatMatMultiply.h"
void MatMatMultiply(const float (&A)[MATRIX_SIZE][MATRIX_SIZE],
    const float (&B)[MATRIX_SIZE][MATRIX_SIZE], float (&C)[MATRIX_SIZE][MATRIX_SIZE])
    static constexpr int NBLOCKS = MATRIX_SIZE / BLOCK_SIZE;
    using blocked_matrix_t = float (&) [NBLOCKS][BLOCK_SIZE][NBLOCKS][BLOCK_SIZE];
    using const_blocked_matrix_t = const float (&) [NBLOCKS][BLOCK_SIZE][NBLOCKS][BLOCK_SIZE];
    auto blockA = reinterpret_cast<const_blocked_matrix_t>(A[0][0]);
    auto blockB = reinterpret_cast<const_blocked_matrix_t>(B[0][0]);
    auto blockC = reinterpret_cast<blocked_matrix_t>(C[0][0]);
#pragma omp parallel for
    for (int i = 0; i < NBLOCKS; i++)
                                                Adjusting our implementation to a "blocked"
    for (int j = 0; j < NBLOCKS; j++)
                                                       concept of matrix-matrix multiply
        C[i][j] = 0.;
    for (int bi = 0; bi < NBLOCKS; bi++)
    for (int bj = 0; bj < NBLOCKS; bj++)
        for (int bk = 0; bk < NBLOCKS; bk++) {
#pragma omp parallel for
            for (int ii = 0; ii < BLOCK_SIZE; ii++)
            for (int jj = 0; jj < BLOCK_SIZE; jj++)</pre>
            for (int kk = 0; kk < BLOCK_SIZE; kk++)
                blockC[bi][ii][bj][jj] += blockA[bi][ii][bk][kk] * blockB[bk][kk][bj][jj];
```

Theory of GEMM operation

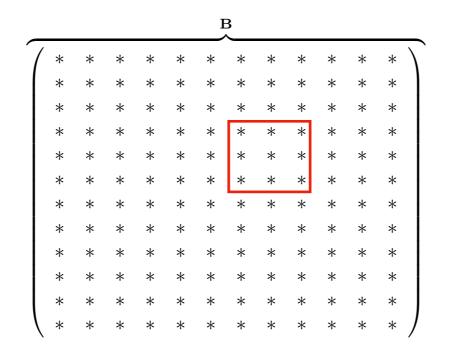


A visual illustration ...

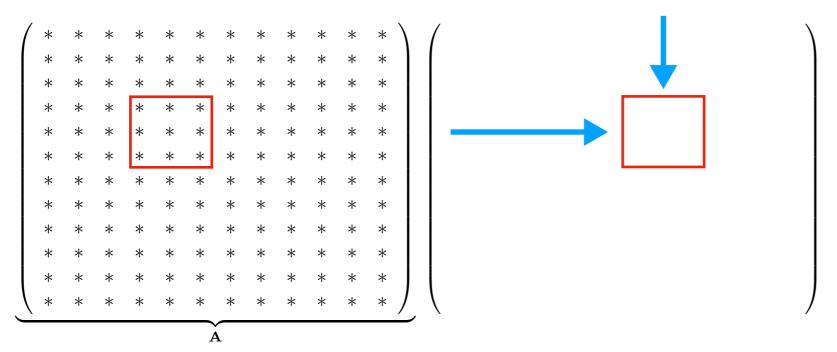


Multiply respective <u>sub-matrices (blocks)</u> of **A** & **B**, accumulate on highlighted <u>block</u> of **C=A*B**

Theory of GEMM operation

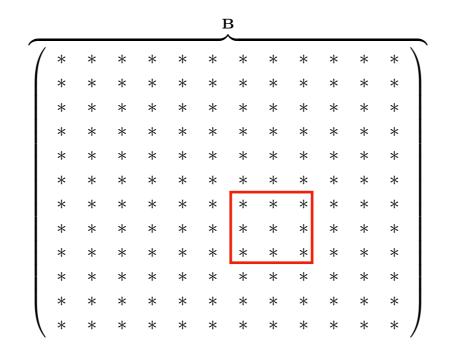


A visual illustration ...

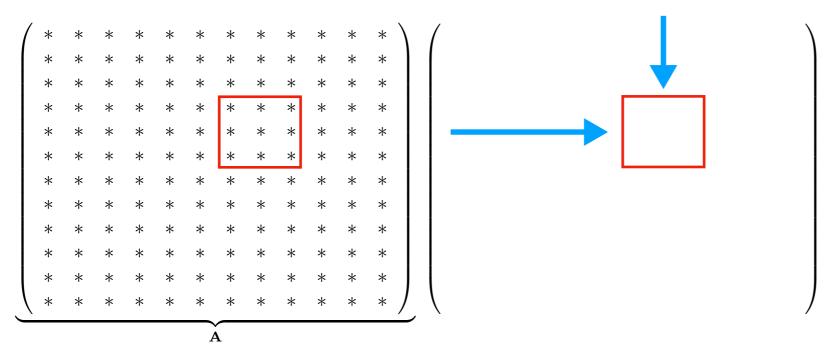


Multiply respective <u>sub-matrices (blocks)</u> of **A** & **B**, accumulate on highlighted <u>block</u> of **C=A*B**

Theory of GEMM operation

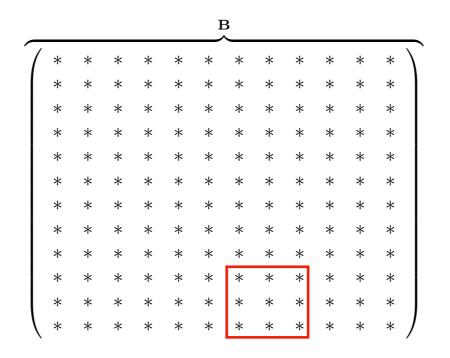


A visual illustration ...



Multiply respective <u>sub-matrices (blocks)</u> of **A** & **B**, accumulate on highlighted <u>block</u> of **C=A*B**

Theory of GEMM operation



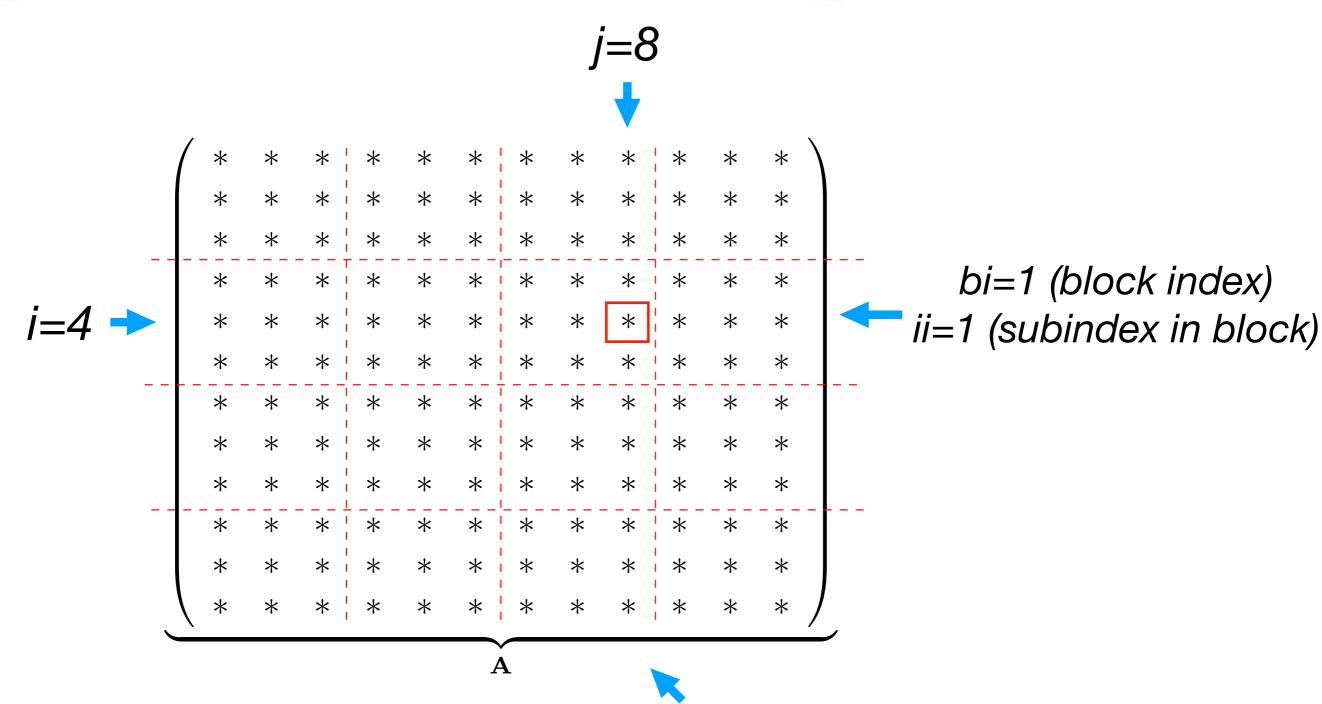
A visual illustration ...

Tiling, blocking promotes cache reuse with a limited working set size

$$\begin{array}{c} \texttt{for} \ i = 1 \dots N \\ \\ \texttt{for} \ j = 1 \dots N \\ \\ C_{ij} \leftarrow 0 \\ \\ \texttt{for} \ k = 1 \dots N \\ \\ C_{ij} \leftarrow C_{ij} + A_{ik}B_{kj} \end{array}$$

Here Cij, Aik, and Bkj denote matrix blocks

"Blocked" indexing of matrix entries



bj=2 (block index) jj=2 (subindex in block)

GEMM routine (MatMatMultiply.cpp) | DenseAlgebra/GEMM_Test_0_2|

```
#include "MatMatMultiply.h"
void MatMatMultiply(const float (&A)[MATRIX_SIZE][MATRIX_SIZE],
    const float (&B)[MATRIX_SIZE][MATRIX_SIZE], float (&C)[MATRIX_SIZE][MATRIX_SIZE])
{
    static constexpr int NBLOCKS = MATRIX_SIZE / BLOCK_SIZE;
    using blocked_matrix_t = float (&) [NBLOCKS][BLOCK_SIZE][NBLOCKS][BLOCK_SIZE];
    using const_blocked_matrix_t = const float (&) [NBLOCKS][BLOCK_SIZE][NBLOCKS][BLOCK_SIZE];
    auto blockA = reinterpret_cast<const_blocked_matrix_t>(A[0][0]);
    auto blockB = reinterpret_cast<const_blocked_matrix_t>(B[0][0]);
    auto blockC = reinterpret_cast<blocked_matrix_t>(C[0][0]);
#pragma omp parallel for
                                            Cast matrices such that they can be indexed
    for (int i = 0; i < NBLOCKS; i++)
    for (int j = 0; j < NBLOCKS; j++)
                                                    using four numbers as follows:
        C[i][j] = 0.;
                                          [row block][row subindex][col block][col subindex]
    for (int bi = 0; bi < NBLOCKS; bi++)
    for (int bj = 0; bj < NBLOCKS; bj++)
        for (int bk = 0; bk < NBLOCKS; bk++) {
#pragma omp parallel for
            for (int ii = 0; ii < BLOCK_SIZE; ii++)
            for (int jj = 0; jj < BLOCK_SIZE; jj++)</pre>
            for (int kk = 0; kk < BLOCK_SIZE; kk++)
                blockC[bi][ii][bj][jj] += blockA[bi][ii][bk][kk] * blockB[bk][kk][bj][jj];
```



GEMM routine (MatMatMultiply.cpp) | DenseAlgebra/GEMM_Test_0_2|

```
#include "MatMatMultiply.h"
void MatMatMultiply(const float (&A)[MATRIX_SIZE][MATRIX_SIZE],
    const float (&B)[MATRIX_SIZE][MATRIX_SIZE], float (&C)[MATRIX_SIZE][MATRIX_SIZE])
    static constexpr int NBLOCKS = MATRIX_SIZE / BLOCK_SIZE;
    using blocked_matrix_t = float (&) [NBLOCKS][BLOCK_SIZE][NBLOCKS][BLOCK_SIZE];
    using const_blocked_matrix_t = const float (&) [NBLOCKS][BLOCK_SIZE][NBLOCKS][BLOCK_SIZE];
    auto blockA = reinterpret_cast<const_blocked_matrix_t>(A[0][0]);
    auto blockB = reinterpret_cast<const_blocked_matrix_t>(B[0][0]);
    auto blockC = reinterpret_cast<blocked_matrix_t>(C[0][0]);
#pragma omp parallel for
    for (int i = 0; i < NBLOCKS; i++)
    for (int j = 0; j < NBLOCKS; j++)
        C[i][j] = 0.;
    for (int bi = 0; bi < NBLOCKS; bi++)
    for (int bj = 0; bj < NBLOCKS; bj++)
        for (int bk = 0; bk < NBLOCKS; bk++) {
#pragma omp parallel for
            for (int ii = 0; ii < BLOCK_SIZE; ii++)
                                                     Use 6-way (instead of 3-way) for-loop
            for (int jj = 0; jj < BLOCK_SIZE; jj++)</pre>
            for (int kk = 0; kk < BLOCK_SIZE; kk++)
                blockC[bi][ii][bj][jj] += blockA[bi][ii][bk][kk] * blockB[bk][kk][bj][jj];
```



GEMM routine (MatMatMultiply.cpp) | DenseAlgebra/GEMM_Test_0_2

```
#include "MatMatMultiply.h"
void MatMatMultiply(const float (&A)[MATRIX_SIZE][MATRIX_SIZE],
    const float (&B)[MATRIX_SIZE][MATRIX_SIZE], float (&C)[MATRIX_SIZE][MATRIX_SIZE])
    static constexpr int NBLOCKS = MATRIX_SIZE / BLOCK_SIZE;
    using blocked_matrix_t = float (&) [NBLOCKS][BLOCK_SIZE][NBLOCKS][BLOCK_SIZE];
    using const_blocked_matrix_t = const float (&) [NBLOCKS][BLOCK_SIZE][NBLOCKS][BLOCK_SIZE];
    auto blockA = reinterpret_cast<const_blocked_matrix_t>(A[0][0]);
    auto blockB = reinterpret_cast<const_blocked_matrix_t>(B[0][0]);
    auto blockC = reinterpret_cast<blocked_matrix_t>(C[0][0]);
#pragma omp parallel for
                                                             At matrix size = 1024
    for (int i = 0; i < NBLOCKS; i++)
    for (int j = 0; j < NBLOCKS; j++)
        C[i][j] = 0.;
                                                               Execution:
                                          Running test iteration
                                                                  1 [Elapsed time : 171.81ms]
    for (int bi = 0; bi < NBLOCKS; bi++)
                                          Running test iteration 2 [Elapsed time: 134.102ms]
    for (int bj = 0; bj < NBLOCKS; bj++)</pre>
        for (int bk = 0; bk < NBLOCKS; bk+Running test iteration 3 [Elapsed time : 133.837ms]
                                          Running test iteration 4 [Elapsed time: 134.035ms]
                                          Running test iteration
                                                                  5 [Elapsed time : 134.137ms]
#pragma omp parallel for
            for (int ii = 0; ii < BLOCK_SI Running test iteration 6 [Elapsed time : 139.447ms]
            for (int jj = 0; jj < BLOCK_SI Running test iteration 7 [Elapsed time : 133.784ms]
            for (int kk = 0; kk < BLOCK_SI Running test iteration
                                                                  8 [Elapsed time : 134.448ms]
                blockC[bi][ii][bj][jj] += |Running test iteration
                                                                  9 [Elapsed time : 134.428ms]
                                          Running test iteration 10 [Elapsed time: 164.302ms]
```

 $[\ldots]$

```
Correctness checking logic
#include "MatMatMultiply.h"
#include "Timer.h"
#include "Utilities.h"
#include <iostream>
#include <iomanip>
int main(int argc, char *argv□)
    float *Araw =
        static_cast<float*>( AlignedAllocate( MATRIX_SIZE * MATRIX_SIZE * sizeof(float), 64 ) );
    float *Braw =
        static_cast<float*>( AlignedAllocate( MATRIX_SIZE * MATRIX_SIZE * sizeof(float), 64 ) );
    float *Craw =
        static_cast<float*>( AlignedAllocate( MATRIX_SIZE * MATRIX_SIZE * sizeof(float), 64 ) );
    float *referenceCraw =
        static_cast<float*>( AlignedAllocate( MATRIX_SIZE * MATRIX_SIZE * sizeof(float), 64 ) );
    using matrix_t = float (&) [MATRIX_SIZE][MATRIX_SIZE];
    matrix_t A = reinterpret_cast<matrix_t>(*Araw);
    matrix_t B = reinterpret_cast<matrix_t>(*Braw);
    matrix_t C = reinterpret_cast<matrix_t>(*Craw);
    matrix_t referenceC = reinterpret_cast<matrix_t>(*referenceCraw);
    InitializeMatrices(A, B);
    Timer timer;
```

LDenseAlgebra/GEMM_Test_0_31

#include "MatMatMultiply.h"

#include "Timer.h"

```
#include "Utilities.h"
#include <iostream>
#include <iomanip>
int main(int argc, char *argv□)
    float *Araw =
    float *Braw =
    float *Craw =
    float *referenceCraw =
    InitializeMatrices(A, B);
    Timer timer;
    [\ldots]
```

```
LDenseAlgebra/GEMM_Test_0_31
```

Very Important:

```
Build infrastructure for testing correctness
                                        before implementing code transformations
   static_cast<float*>( AlignedAllocate( MATRIX_SIZE * MATRIX_SIZE * sizeof(float), 64 ) );
   static_cast<float*>( AlignedAllocate( MATRIX_SIZE * MATRIX_SIZE * sizeof(float), 64 ) );
   static_cast<float*>( AlignedAllocate( MATRIX_SIZE * MATRIX_SIZE * sizeof(float), 64 ) );
   static_cast<float*>( AlignedAllocate( MATRIX_SIZE * MATRIX_SIZE * sizeof(float), 64 ) );
using matrix_t = float (&) [MATRIX_SIZE][MATRIX_SIZE];
matrix_t A = reinterpret_cast<matrix_t>(*Araw);
matrix_t B = reinterpret_cast<matrix_t>(*Braw);
matrix_t C = reinterpret_cast<matrix_t>(*Craw);
matrix_t referenceC = reinterpret_cast<matrix_t>(*referenceCraw);
```

return 0;

```
DenseAlgebra/GEMM_Test_0_3
```

```
Very Important:
int main(int argc, char *argv[])
                                                 Build infrastructure for testing correctness
{
    [...]
                                                before implementing code transformations
    // Correctness test
    std::cout << "Running candidate kernel for correctness test ... " << std::flush;</pre>
    timer.Start();
    MatMatMultiply(A, B, C);
    timer.Stop("Elapsed time : ");
    std::cout << "Running reference kernel for correctness test ... " << std::flush;</pre>
    timer.Start();
    MatMatMultiplyReference(A, B, reference(C);
    timer.Stop("Elapsed time : ");
    float discrepancy = MatrixMaxDifference(C, referenceC);
    std::cout << "Discrepancy between two methods : " << discrepancy << std::endl;</pre>
    for(int test = 1; test <= 20; test++)
        std::cout << "Running kernel for performance run #" << std::setw(2) << test << " ... ";</pre>
        timer.Start();
        MatMatMultiply(A, B, C);
        timer.Stop("Elapsed time : ");
    }
```

GEMM routine (MatMatMultiply.h)

```
DenseAlgebra/GEMM_Test_0_3
```

The "reference" implementation is using MKL BLAS

(the "non-reference" is our hand-built version,

with any transformations we enact)

GEMM routine (MatMatMultiply.cpp) DenseAlgebra/GEMM_Test_0_3

```
#include "MatMatMultiply.h"
#include "mkl.h"
void MatMatMultiply(const float (&A)[MATRIX_SIZE][MATRIX_SIZE],
    const float (&B)[MATRIX_SIZE][MATRIX_SIZE], float (&C)[MATRIX_SIZE][MATRIX_SIZE])
#pragma omp parallel for
    for (int i = 0; i < MATRIX_SIZE; i++)
    for (int j = 0; j < MATRIX_SIZE; j++) {
        C[i][j] = 0.;
        for (int k = 0; k < MATRIX_SIZE; k++)
            C[i][j] += A[i][k] * B[k][j];
void MatMatMultiplyReference(const float (&A)[MATRIX_SIZE][MATRIX_SIZE],
    const float (&B)[MATRIX_SIZE][MATRIX_SIZE], float (&C)[MATRIX_SIZE][MATRIX_SIZE])
    cblas_sgemm(
        CblasRowMajor, CblasNoTrans, CblasNoTrans,
        MATRIX_SIZE, MATRIX_SIZE, MATRIX_SIZE,
        1.,
        &A[0][0], MATRIX_SIZE,
        &B[0][0], MATRIX_SIZE,
        0.,
        &C[0][0], MATRIX_SIZE
    );
```

Comparison code (Utilities.cpp)

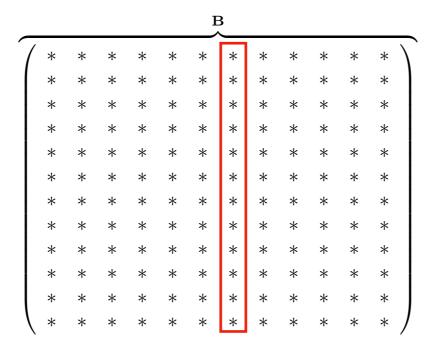
```
DenseAlgebra/GEMM_Test_0_3
```

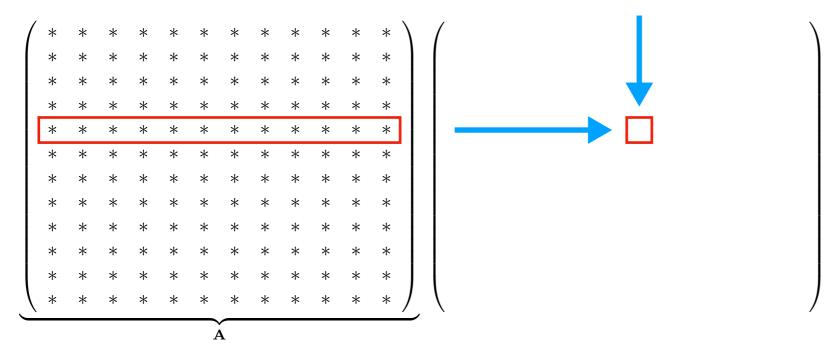
```
float MatrixMaxDifference(const float (&A)[MATRIX_SIZE][MATRIX_SIZE],
    const float (&B)[MATRIX_SIZE][MATRIX_SIZE])
{
    float result = 0.;
    for (int i = 0; i < MATRIX_SIZE; i++)
        for (int j = 0; j < MATRIX_SIZE; j++)
            result = std::max( result, std::abs( A[i][j] - B[i][j] ) );
    return result;
}</pre>
```

DenseAlgebra/GEMM_Test_0_3

```
int main(int argc, char *argv[])
{
    [...]
    // Correctness test
    std::cout << "Running candidate kernel for correctness test ... " << std::flush;</pre>
    timer.Start();
    MatMatMultiply(A, B, C);
    timer.Stop("Elapsed time : ");
    std::cout << "Running reference kernel for correctness test ... " << std::flush;</pre>
    timer.Start();
    MatMatMultiplyReference(A, B, reference();
    timer.Stop("Elapsed time : ");
    float discrepancy = MatrixMaxDifference(C, referenceC);
    std::cout << "Discrepancy between two methods : " << discrepancy << std::endl;</pre>
    for(int test =
                                                     Execution:
                   Running candidate kernel for correctness test ... [Elapsed time : 273.398ms]
        std::cout {Running reference kernel for correctness test ... [Elapsed time : 29.5605ms]
        timer.StartDiscrepancy between two methods: 8.01086e-05
        MatMatMultiRunning kernel for performance run # 1 ... [Elapsed time : 221.153ms]
        timer.Stop(Running kernel for performance run # 2 ... [Elapsed time : 222.238ms]
    }
                   Running kernel for performance run # 3 ... [Elapsed time : 221.794ms]
                   Running kernel for performance run # 4 ... [Elapsed time : 224.306ms]
    return 0;
                   [...]
```

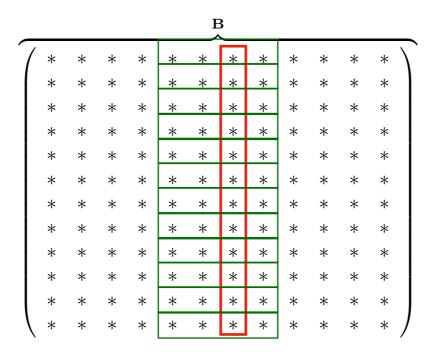
Causes of slowdown

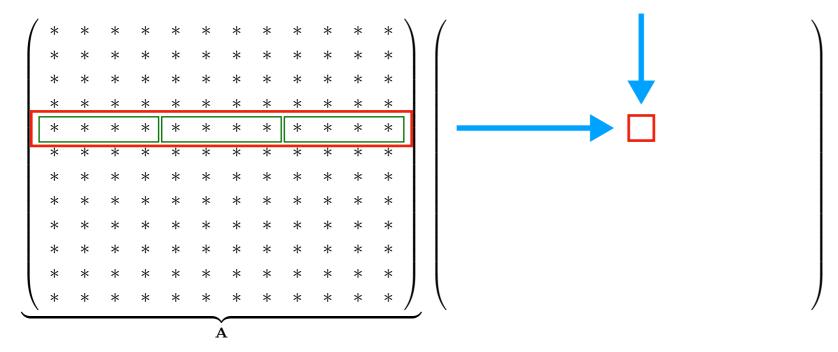




$$ext{for } i = 1 \dots N$$
 $ext{for } j = 1 \dots N$ $ext{} C_{ij} \leftarrow 0$ $ext{for } k = 1 \dots N$ $ext{} C_{ij} \leftarrow C_{ij} + A_{ik} B_{kj}$

Causes of slowdown



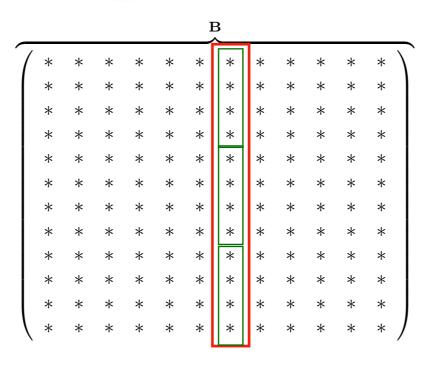


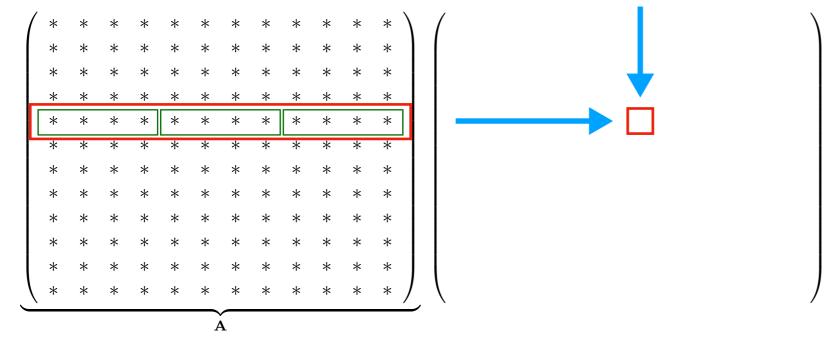
$$\begin{array}{c} \texttt{for} \ i = 1 \dots N \\ \\ \texttt{for} \ j = 1 \dots N \\ \\ C_{ij} \leftarrow 0 \\ \\ \texttt{for} \ k = 1 \dots N \\ \\ C_{ij} \leftarrow C_{ij} + A_{ik}B_{kj} \end{array}$$

Shapes of cache lines (for row-major matrices)

Memory bandwidth is being wasted while reading factor **B** ...

Causes of slowdown



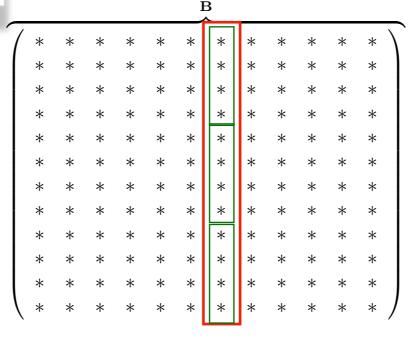


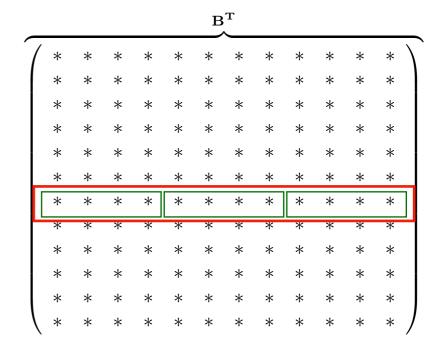
$$\begin{array}{c} \texttt{for} \ i = 1 \dots N \\ \\ \texttt{for} \ j = 1 \dots N \\ \\ C_{ij} \leftarrow 0 \\ \\ \texttt{for} \ k = 1 \dots N \\ \\ C_{ij} \leftarrow C_{ij} + A_{ik}B_{kj} \end{array}$$

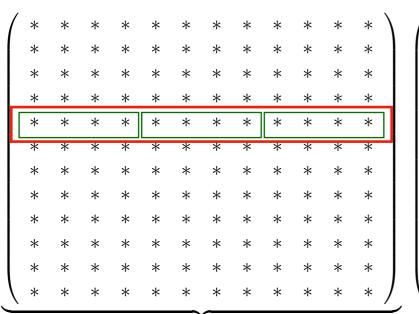
If, instead, **B** was given as column-major ...

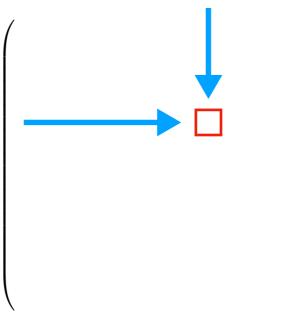
... cache lines are more effectively utilized

Use transpose?



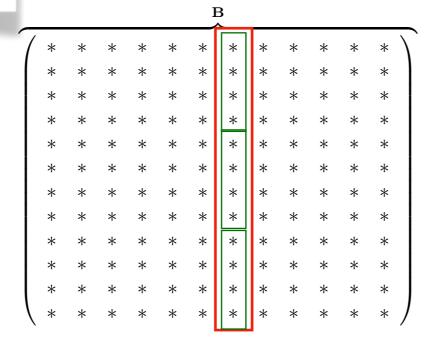


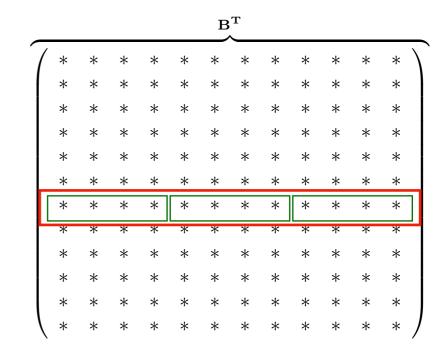


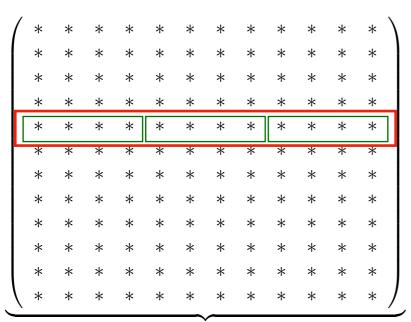


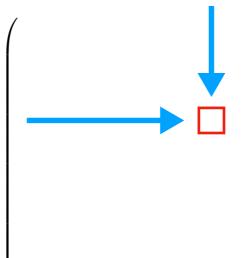
$$\begin{array}{c} \texttt{for} \ i = 1 \dots N \\ \\ \texttt{for} \ j = 1 \dots N \\ \\ C_{ij} \leftarrow 0 \\ \\ \texttt{for} \ k = 1 \dots N \\ \\ C_{ij} \leftarrow C_{ij} + A_{ik}B_{kj} \end{array}$$

Use transpose?









$$\begin{array}{l} \text{for } i=1\dots N \\ \text{for } j=1\dots N \\ C_{ij} \leftarrow 0 \\ \text{for } k=1\dots N \\ C_{ij} \leftarrow C_{ij} + A_{ik} [B^T]_{jk} \end{array}$$

Multiplying with the transpose of B gives better cache utilization!

Two different interpretations:

(1) We multiply with B, stored in <u>column-major</u> format, or (2) We multiply with B^T, stored in <u>row-major</u> format

DenseAlgebra/GEMM_Test_0_4

```
[...]
int main(int argc, char *argv[])
    float *Araw=static_cast<float*>(AlignedAllocate(MATRIX_SIZE*MATRIX_SIZE*sizeof(float),64));
    float *Braw=static_cast<float*>(AlignedAllocate(MATRIX_SIZE*MATRIX_SIZE*sizeof(float),64));
    float *BTraw=static_cast<float*>(AlignedAllocate(MATRIX_SIZE*MATRIX_SIZE*sizeof(float),64));
    float *Craw=static_cast<float*>(AlignedAllocate(MATRIX_SIZE*MATRIX_SIZE*sizeof(float),64));
    [...]
    matrix_t A = reinterpret_cast<matrix_t>(*Araw);
    matrix_t B = reinterpret_cast<matrix_t>(*Braw);
    matrix_t BT = reinterpret_cast<matrix_t>(*BTraw);
    [\ldots]
    InitializeMatrices(A, B);
                                                            Build the matrix B<sup>T</sup> in advance ...
    Timer timer;
                                                           Storage overhead is higher than compute`
    // Pre-transposing B
    std::cout << "Transposing second matrix factor ... " << std::flush;</pre>
    timer.Start();
    MatTranspose(B, BT);
    timer.Stop("Elapsed time : ");
    [\ldots]
```

DenseAlgebra/GEMM_Test_0_4

```
[...]
int main(int argc, char *argv[])
    [...]
    // Correctness test
    std::cout << "Running candidate kernel for correctness test ... " << std::flush;</pre>
    timer.Start();
    MatMatTransposeMultiply(A, BT, C);
    timer.Stop("Elapsed time : ");
    std::cout << "Running reference kernel for correctness test ... " << std::flush;</pre>
    timer.Start();
    MatMatMultiplyReference(A, B, reference(C);
                                                     ... and multiply with the transpose instead
    timer.Stop("Elapsed time : ");
    float discrepancy = MatrixMaxDifference(C, referenceC);
    std::cout << "Discrepancy between two methods : " << discrepancy << std::endl;</pre>
    for(int test = 1; test <= 20; test++)
        std::cout << "Running kernel for performance run #" << std::setw(2) << test << " ... ";</pre>
        timer.Start();
        MatMatTransposeMultiply(A, BT, C);
        timer.Stop("Elapsed time : ");
    }
    return 0;
```

Multiply w/Transpose (MatMatMultiply.cpp)

```
[...]
void MatTranspose(const float (&A)[MATRIX_SIZE][MATRIX_SIZE],
   float (&AT)[MATRIX_SIZE][MATRIX_SIZE])
{
   mkl_somatcopy(
            // Matrix A is in row-major format
        'T', // We are performing a transposition operation
       MATRIX_SIZE, // Dimensions of matrix -- rows ...
       MATRIX_SIZE, // ... and columns
              // No scaling
       &A[0][0], // Input matrix
       MATRIX_SIZE, // Leading dimension (here, just the matrix dimension)
       &AT[0][0], // Output matrix
       MATRIX_SIZE // Leading dimension
    );
void MatMatTransposeMultiply(const float (&A)[MATRIX_SIZE][MATRIX_SIZE],
    const float (&B)[MATRIX_SIZE][MATRIX_SIZE], float (&C)[MATRIX_SIZE][MATRIX_SIZE])
#pragma omp parallel for
   for (int i = 0; i < MATRIX_SIZE; i++)
    for (int j = 0; j < MATRIX_SIZE; j++) {
       C[i][j] = 0.;
       for (int k = 0; k < MATRIX_SIZE; k++)
           C[i][j] += A[i][k] * B[j][k];
```

Multiply w/Transpose (MatMatMultiply.cpp)

```
[...]
void MatTranspose(const float (&A)[MATRIX_SIZE][MATRIX_SIZE],
   float (&AT)[MATRIX_SIZE][MATRIX_SIZE])
{
   mkl_somatcopy(
        'R', // Matrix A is in row-major format
        'T', // We are performing a transposition operation
       MATRIX_SIZE, // Dimensions of matrix -- rows ...
       MATRIX_SIZE, // ... and columns
              // No scaling
       1.,
       &A[0][0], // Input matrix
       MATRIX_SIZE, // Leading dimension (here, just the matrix dimension)
       &AT[0][0], // Output matrix
       MATRIX_SIZE // Leading dimension
    );
void MatMatTransposeMultiply(const float (&A)[MATRIX_SIZE][MATRIX_SIZE],
    const float (&B)[MATRIX_SIZE][MATRIX_SIZE], float (&C)[MATRIX_SIZE][MATRIX_SIZE])
#pragma omp parallel for
   for (int i = 0; i < MATRIX_SIZE; i++)
    for (int j = 0; j < MATRIX_SIZE; j++) {
       C[i][j] = 0.;
       for (int k = 0; k < MATRIX_SIZE; k++)
           C[i][j] += A[i][k] * B[j][k];
```

Multiply w/Transpose (MatMatMultiply.cpp)

```
[...]
void MatTranspose(const float (&A)[MATRIX_SIZE][MATRIX_SIZE],
    float (&AT)[MATRIX_SIZE][MATRIX_SIZE])
{
    mkl_somatcopy(
             // Matrix A is in row-major format
        'T', // We are performing a transposition operation
        MATRIX_SIZE, // Dimensions of matrix -- rows ...
        MATRIX_SIZE, // ... and columns
               // No scaling
        &A[0][0], // Input matrix
        MATRIX_SIZE, // Leading dimension (here, just the matrix dimension)
        &AT[0][0], // Output matrix
       MATRIX_SIZE // Leading dimension
    );
void MatMatTransposeMultiply(const float (&A)[MATRIX_SIZE][MATRIX_SIZE],
    const float (&B)[MATRIX_SIZE][MATRIX_SIZE], float (&C)[MATRIX_SIZE][MATRIX_SIZE])
#pragma omp parallel for
                                                         for i = 1 \dots N
    for (int i = 0; i < MATRIX_SIZE; i++)
    for (int j = 0; j < MATRIX_SIZE; j++) {
                                                             for j = 1 \dots N
        C[i][j] = 0.;
                                                                C_{ij} \leftarrow 0
        for (int k = 0; k < MATRIX_SIZE; k++)
            C[i][j] += A[i][k] * B[j][k];
                                                                 for k = 1 \dots N
                                                                    C_{ij} \leftarrow C_{ij} + A_{ik}[B^T]_{jk}
```

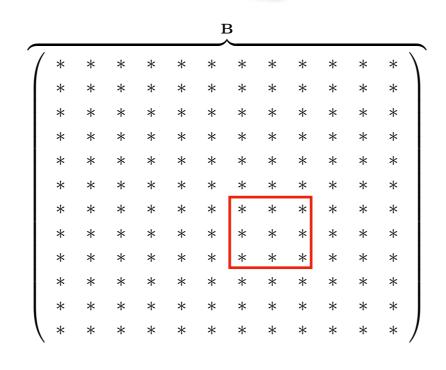
Multiply w/Transpose (MatMatMultiply.cpp)

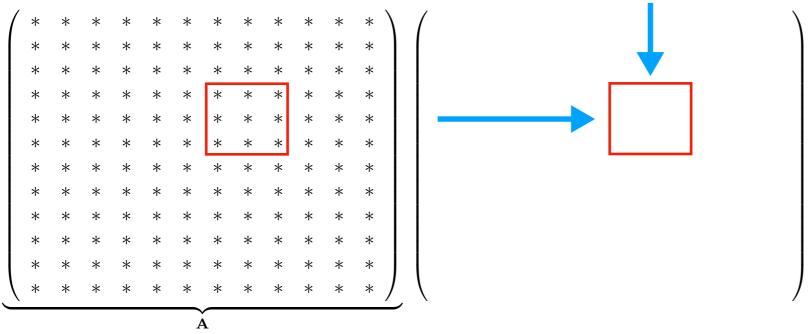
```
[...]
void MatTranspose(const float (&A)[MATRIX_SIZE][MATRIX_SIZE],
    float (&AT)[MATRIX_SIZE][MATRIX_SIZE])
{
   mkl_somatcopy(
        'R',
             // Matrix A is in row-major format
        'T', // We are performing a transposition operation
       MATRIX_SIZE, // Dimensions of matrix -- rows ...
       MATRIX_SIZE, // ... and columns
                // No scaling
       &A[0][0], // Input matrix
       MATRIX_SIZE, // Leading dimension (here, just the matrix dimension)
       &AT[0][0], // Output matrix
                                                                    At matrix size = 1024
       MATRIX_SIZE // Leading dimension
    );
                                                  Execution:
                  Transposing second matrix factor ... [Elapsed time : 16.4232ms]
void MatMatTranspoRunning candidate kernel for correctness test ... [Elapsed time : 45.558ms]
    const float (& Running reference kernel for correctness test ... [Elapsed time : 1.96817ms]
                  Discrepancy between two methods: 6.86646e-05
#pragma omp parallRunning kernel for performance run # 1 ... [Elapsed time : 34.7349ms]
    for (int i = 0Running kernel for performance run # 2 ... [Elapsed time : 35.4725ms]
    for (int j = 0Running kernel for performance run # 3 ... [Elapsed time : 37.0109ms]
       C[i][j] = Running kernel for performance run # 4 ... [Elapsed time : 36.4638ms]
       for (int kRunning kernel for performance run # 5 ... [Elapsed time : 36.53ms]
           C[i][jRunning kernel for performance run # 6 ... [Elapsed time : 36.6595ms]
                  Running kernel for performance run # 7 ... [Elapsed time : 36.5089ms]
                  [\ldots]
```

Multiply w/Transpose (MatMatMultiply.cpp)

```
[...]
void MatTranspose(const float (&A)[MATRIX_SIZE][MATRIX_SIZE],
    float (&AT)[MATRIX_SIZE][MATRIX_SIZE])
{
   mkl_somatcopy(
        'R',
             // Matrix A is in row-major format
        'T', // We are performing a transposition operation
       MATRIX_SIZE, // Dimensions of matrix -- rows ...
       MATRIX_SIZE, // ... and columns
                // No scaling
       &A[0][0], // Input matrix
       MATRIX_SIZE, // Leading dimension (here, just the matrix dimension)
       &AT[0][0], // Output matrix
                                                                    At matrix size = 2048
       MATRIX_SIZE // Leading dimension
    );
                                                  Execution:
                  Transposing second matrix factor ... [Elapsed time : 28.3228ms]
void MatMatTranspoRunning candidate kernel for correctness test ... [Elapsed time : 413.998ms]
    const float (& Running reference kernel for correctness test ... [Elapsed time : 16.1733ms]
                  Discrepancy between two methods: 0.000152588
#pragma omp parallRunning kernel for performance run # 1 ... [Elapsed time : 391.771ms]
    for (int i = 0Running kernel for performance run # 2 ... [Elapsed time : 394.115ms]
    for (int j = 0Running kernel for performance run # 3 ... [Elapsed time : 395.299ms]
       C[i][j] = Running kernel for performance run # 4 ... [Elapsed time : 388.921ms]
       for (int kRunning kernel for performance run # 5 ... [Elapsed time : 396.476ms]
           C[i][jRunning kernel for performance run # 6 ... [Elapsed time : 403.584ms]
                  Running kernel for performance run # 7 ... [Elapsed time : 396.318ms]
                  [\ldots]
```

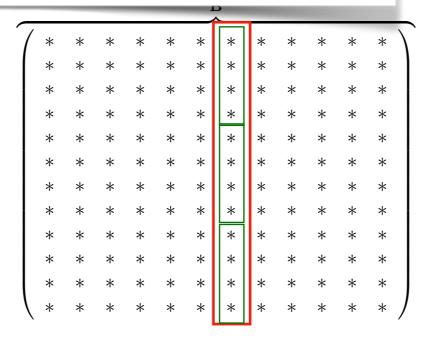
Promising leads: Blocking?

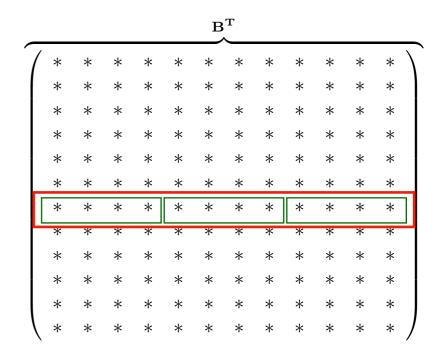


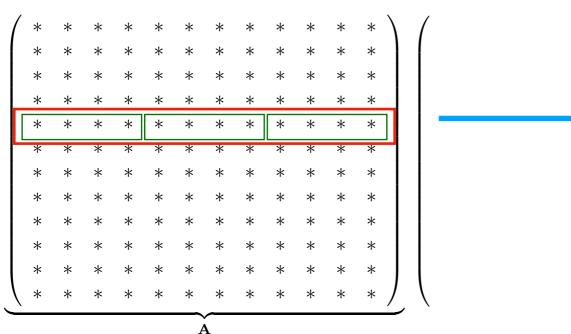


Multiply respective <u>sub-matrices (blocks)</u> of **A** & **B**, accumulate on highlighted <u>block</u> of **C=A*B**

Promising leads: Use transpose?



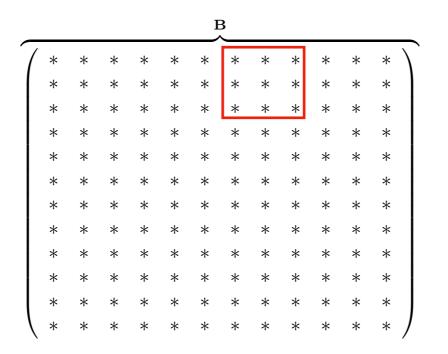


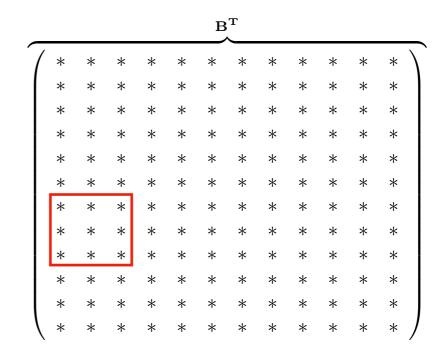


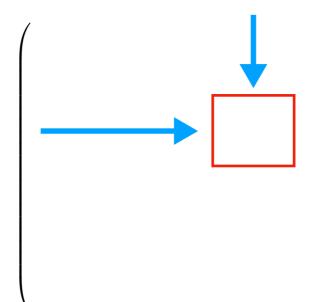
$$\begin{aligned} \text{for } i &= 1 \dots N \\ \text{for } j &= 1 \dots N \\ C_{ij} &\leftarrow 0 \\ \text{for } k &= 1 \dots N \\ C_{ij} &\leftarrow C_{ij} + A_{ik} [B^T]_{jk} \end{aligned}$$

Two different interpretations:

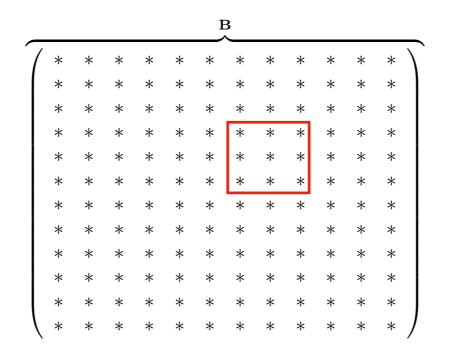
(1) We multiply with B, stored in <u>column-major</u> format, or (2) We multiply with B^T, stored in <u>row-major</u> format

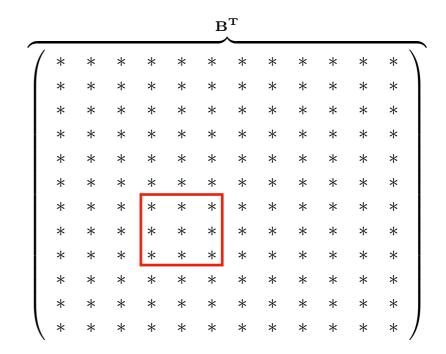


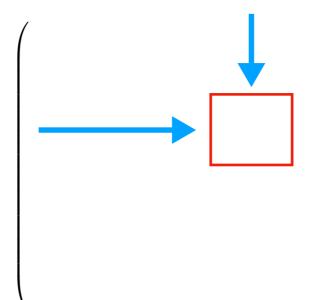




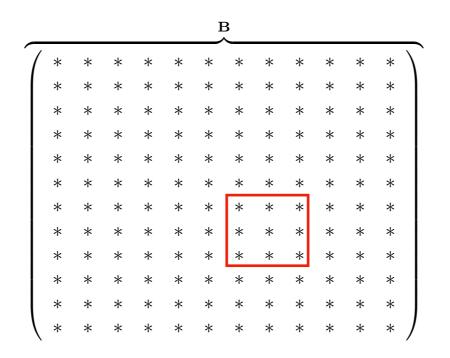
$$\begin{aligned} \text{for } i &= 1 \dots N \\ \text{for } j &= 1 \dots N \\ C_{ij} &\leftarrow 0 \\ \text{for } k &= 1 \dots N \\ C_{ij} &\leftarrow C_{ij} + A_{ik} [B^T]_{jk} \end{aligned}$$

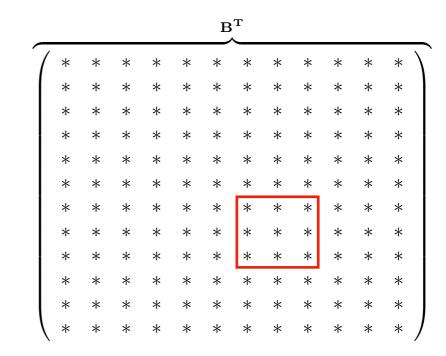


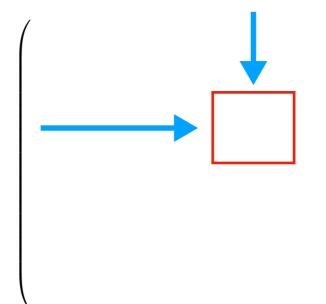




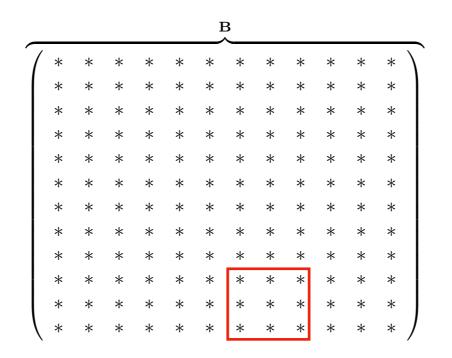
$$\begin{aligned} \text{for } i &= 1 \dots N \\ \text{for } j &= 1 \dots N \\ C_{ij} &\leftarrow 0 \\ \text{for } k &= 1 \dots N \\ C_{ij} &\leftarrow C_{ij} + A_{ik} [B^T]_{jk} \end{aligned}$$

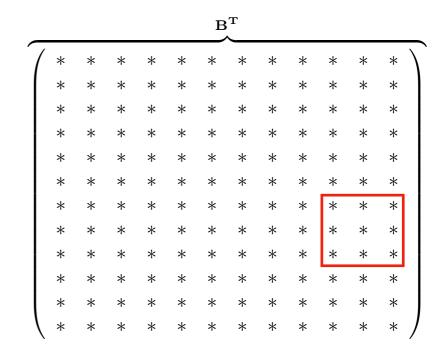


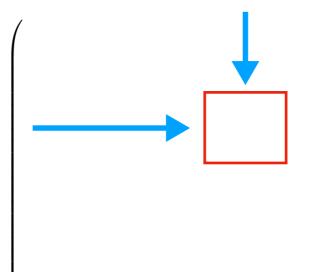




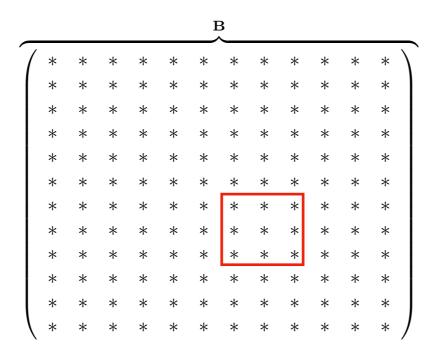
$$\begin{aligned} \text{for } i &= 1 \dots N \\ \text{for } j &= 1 \dots N \\ C_{ij} &\leftarrow 0 \\ \text{for } k &= 1 \dots N \\ C_{ij} &\leftarrow C_{ij} + A_{ik}[B^T]_{jk} \end{aligned}$$

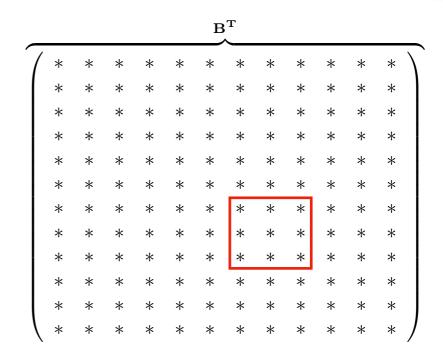


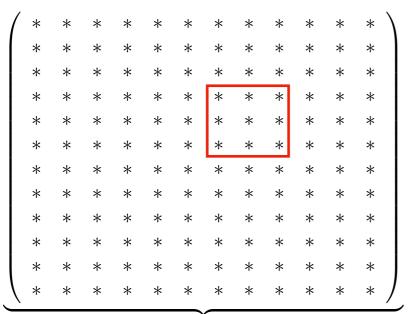


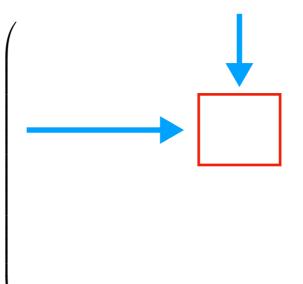


$$\begin{aligned} \text{for } i &= 1 \dots N \\ \text{for } j &= 1 \dots N \\ C_{ij} &\leftarrow 0 \\ \text{for } k &= 1 \dots N \\ C_{ij} &\leftarrow C_{ij} + A_{ik} [B^T]_{jk} \end{aligned}$$

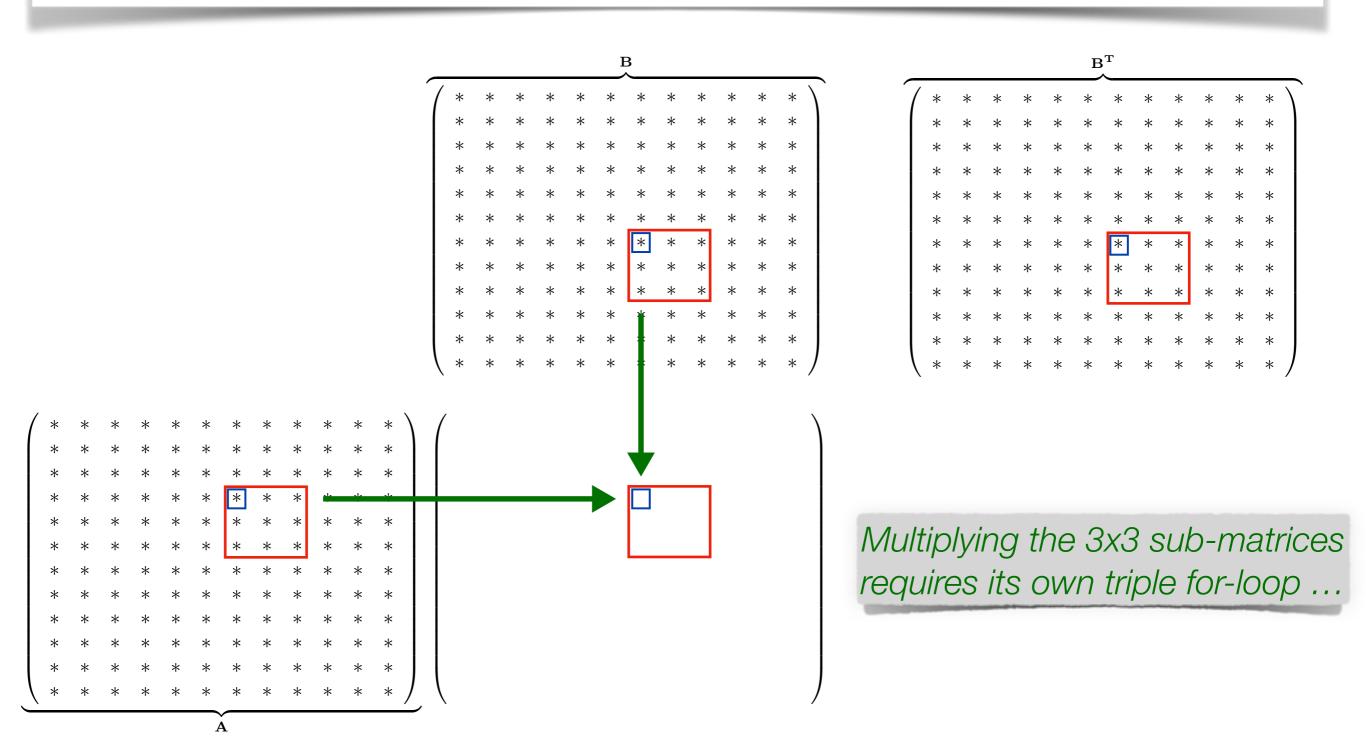


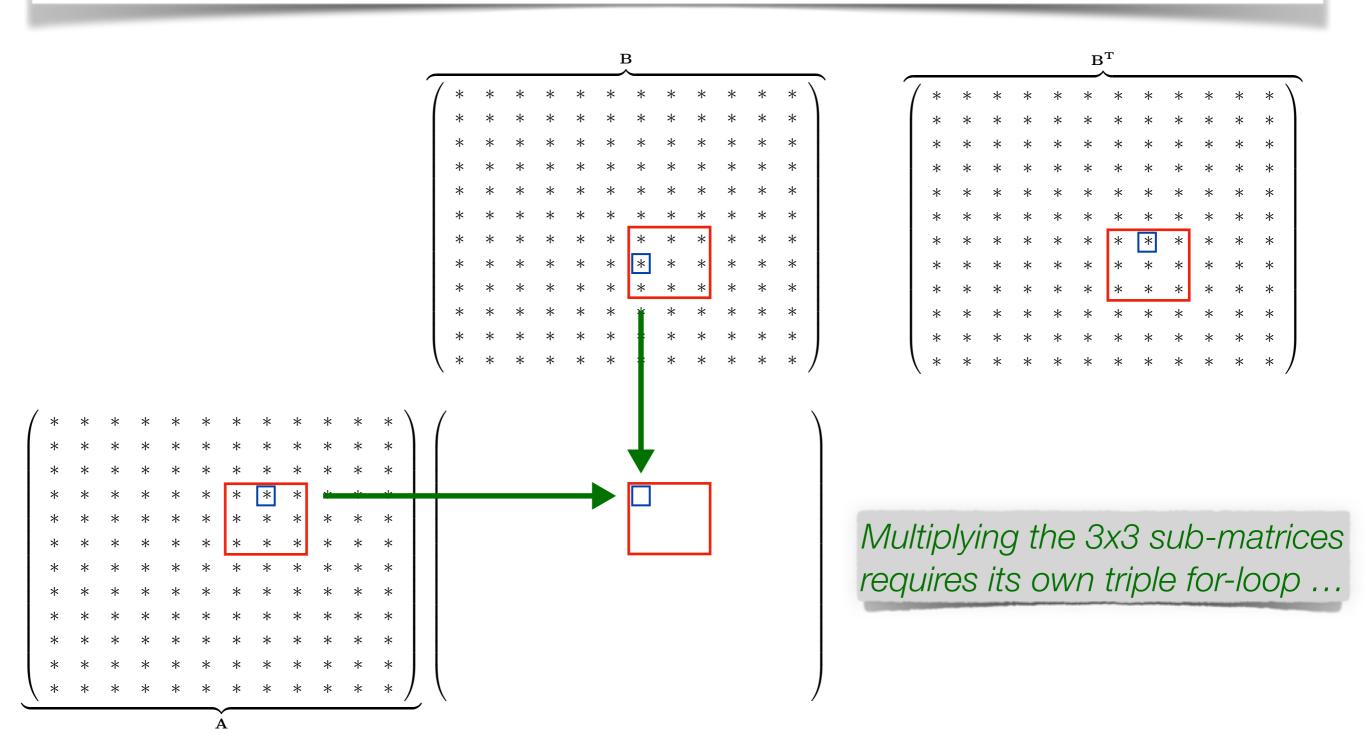


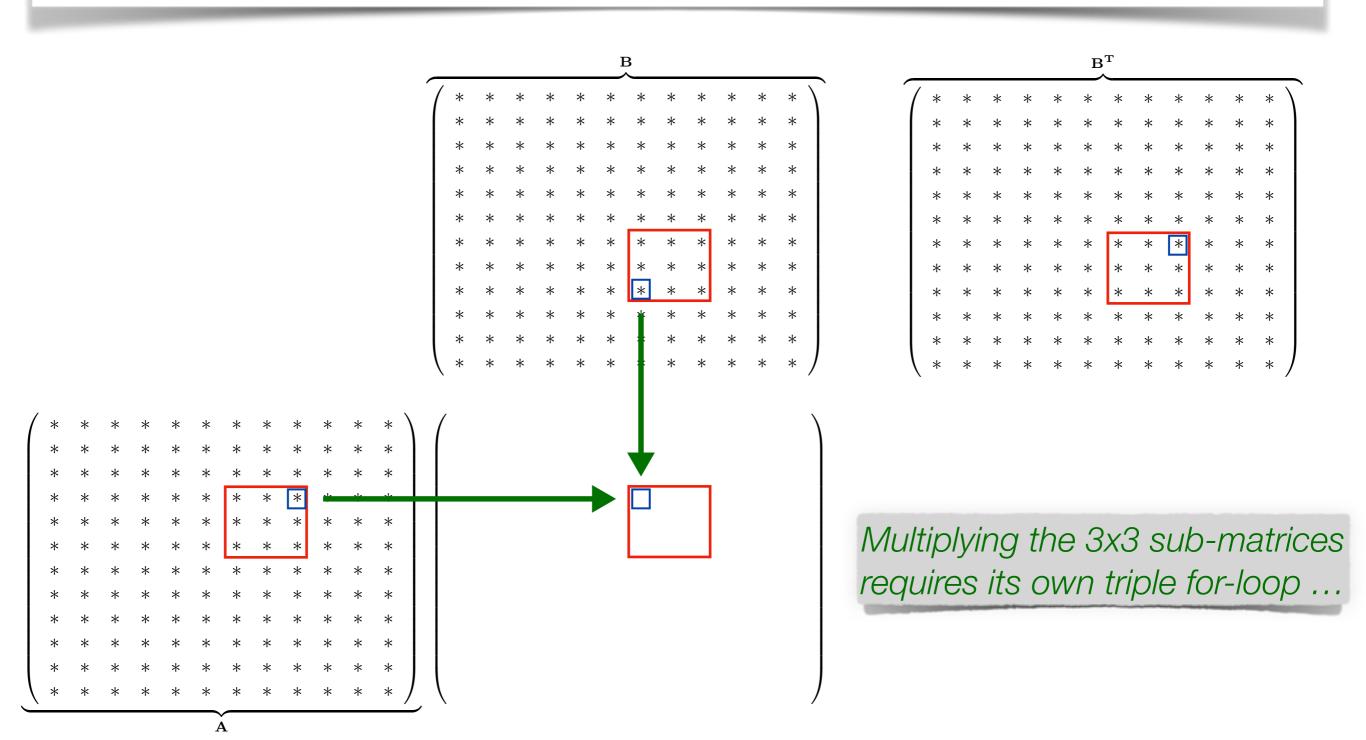


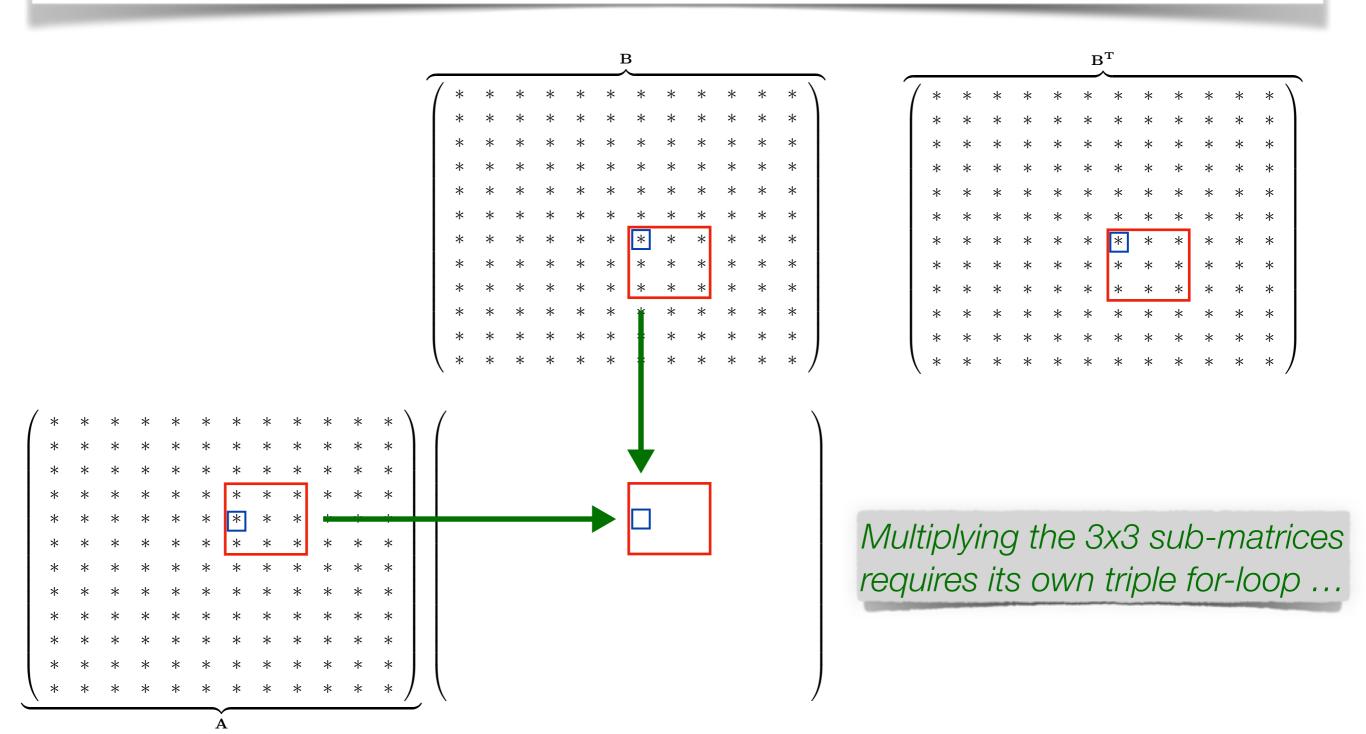


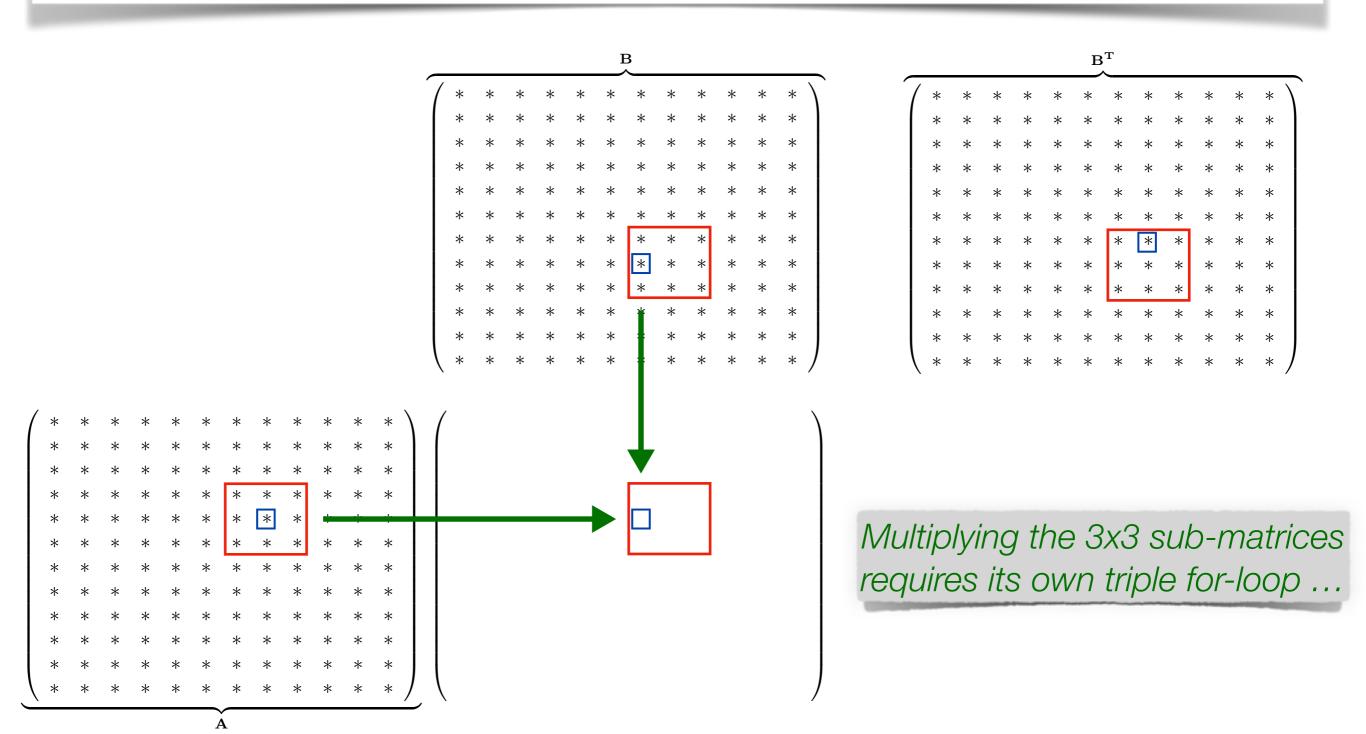
Multiplying the 3x3 sub-matrices requires its own triple for-loop ...

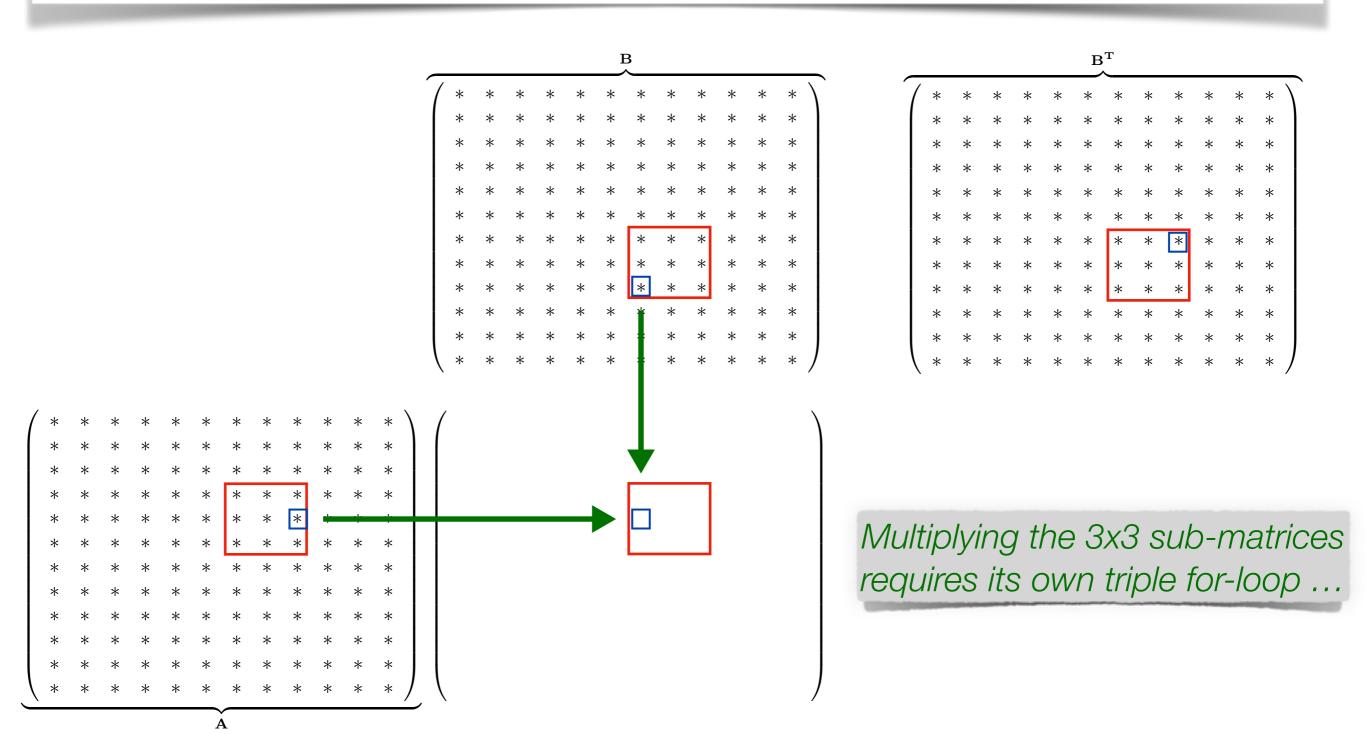


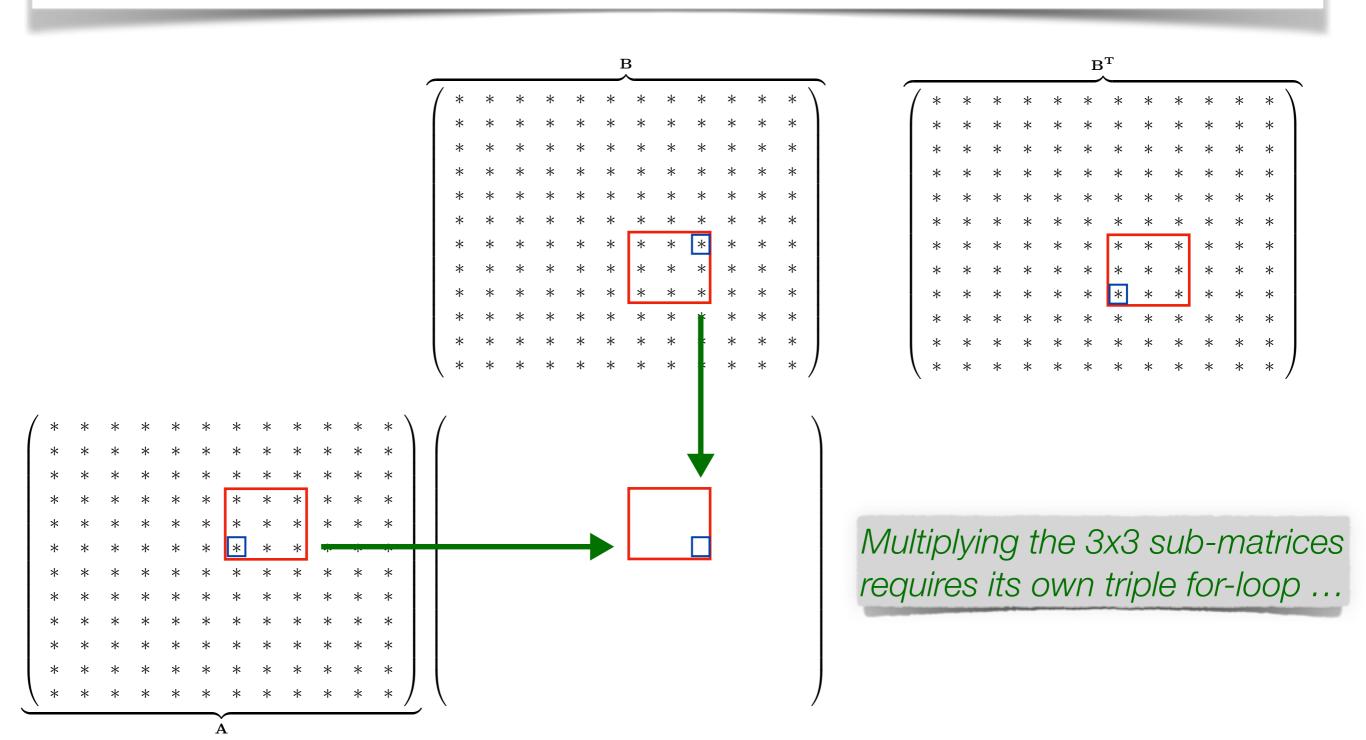


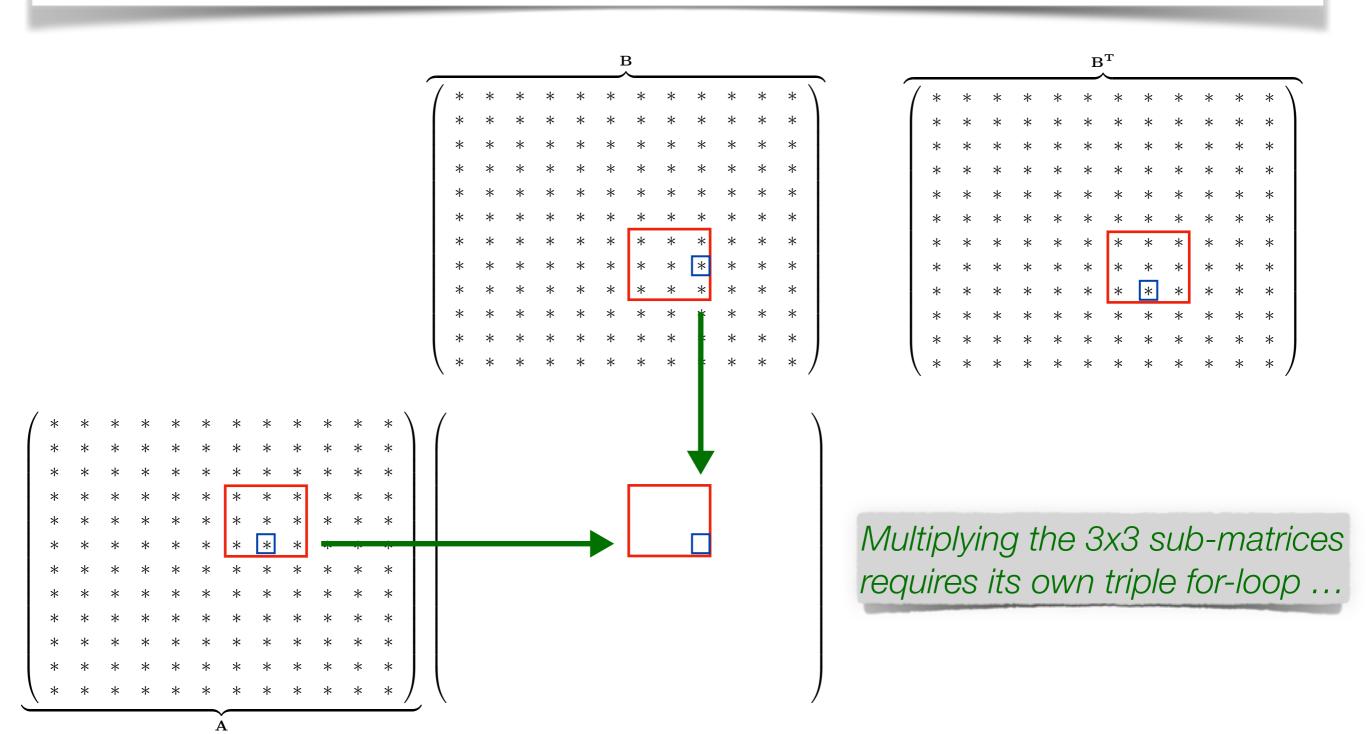


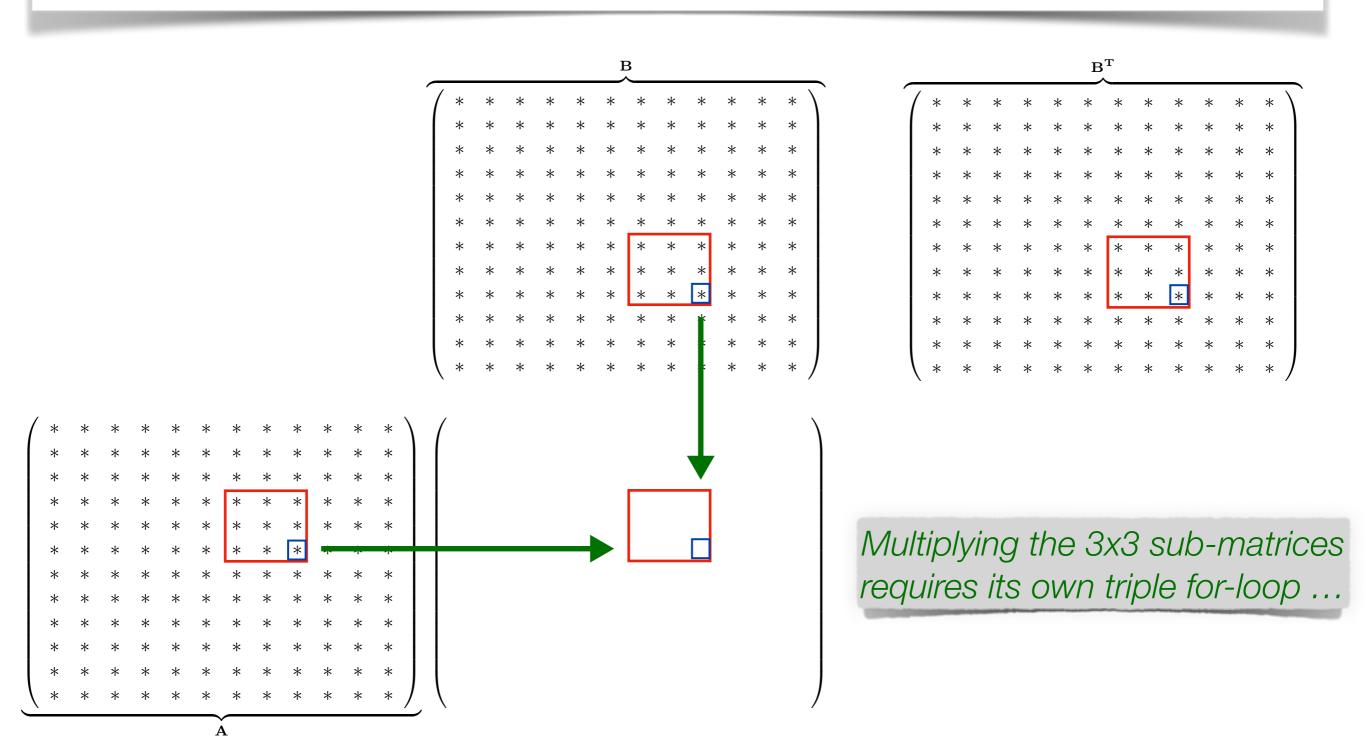












Kernel parameters (Parameters.h)

DenseAlgebra/GEMM_Test_0_5

```
#pragma once

#ifndef MATRIX_SIZE
#define MATRIX_SIZE 1024
#endif

#ifndef BLOCK_SIZE
#define BLOCK_SIZE 32
#endif
```

Kernel parameters (Parameters.h)

DenseAlgebra/GEMM_Test_0_5

```
#pragma once

#ifndef MATRIX_SIZE
#define MATRIX_SIZE 1024
#endif

#ifndef BLOCK_SIZE
#define BLOCK_SIZE
#define BLOCK_SIZE 32
#endif
```

We presume we know, at compile-time, both the matrix size and the size of the sub-matrix blocks

Kernel parameters (Parameters.h)

DenseAlgebra/GEMM_Test_0_5

```
#pragma once

#ifndef MATRIX_SIZE
#define MATRIX_SIZE 1024
#endif

#ifndef BLOCK_SIZE
#define BLOCK_SIZE
#define BLOCK_SIZE 32
#endif
```

#define guards make it easy to override dimensions via compiler options, for testing (e.g. -DMATRIX_SIZE=1024 -DBLOCK_SIZE=32)

GEMM routine (MatMatMultiply.cpp) | DenseAlgebra/GEMM_Test_0_5

```
#include "MatMatMultiply.h"
[\ldots]
void MatMatTransposeMultiply(const float (&A)[MATRIX_SIZE][MATRIX_SIZE],
    const float (&B)[MATRIX_SIZE][MATRIX_SIZE], float (&C)[MATRIX_SIZE][MATRIX_SIZE])
    static constexpr int NBLOCKS = MATRIX_SIZE / BLOCK_SIZE;
    using blocked_matrix_t = float (&) [NBLOCKS][BLOCK_SIZE][NBLOCKS][BLOCK_SIZE];
    using const_blocked_matrix_t = const float (&) [NBLOCKS][BLOCK_SIZE][NBLOCKS][BLOCK_SIZE];
    auto blockA = reinterpret_cast<const_blocked_matrix_t>(A[0][0]);
    auto blockB = reinterpret_cast<const_blocked_matrix_t>(B[0][0]);
    auto blockC = reinterpret_cast<blocked_matrix_t>(C[0][0]);
    for (int i = 0; i < MATRIX_SIZE; i++)
    for (int j = 0; j < MATRIX_SIZE; j++)
        C[i][i] = 0.;
    for (int bi = 0; bi < NBLOCKS; bi++)
    for (int bj = 0; bj < NBLOCKS; bj++)
        for (int bk = 0; bk < NBLOCKS; bk++)
            for (int ii = 0; ii < BLOCK_SIZE; ii++)
            for (int jj = 0; jj < BLOCK_SIZE; jj++)
                for (int kk = 0; kk < BLOCK_SIZE; kk++)
                    blockC[bi][ii][bj][jj] += blockA[bi][ii][bk][kk] * blockB[bj][jj][bk][kk];
```

GEMM routine (MatMatMultiply.cpp) | DenseAlgebra/GEMM_Test_0_5

```
#include "MatMatMultiply.h"
[\ldots]
void MatMatTransposeMultiply(const float (&A)[MATRIX_SIZE][MATRIX_SIZE],
    const float (&B)[MATRIX_SIZE][MATRIX_SIZE], float (&C)[MATRIX_SIZE][MATRIX_SIZE])
    static constexpr int NBLOCKS = MATRIX_SIZE / BLOCK_SIZE;
    using blocked_matrix_t = float (&) [NBLOCKS][BLOCK_SIZE][NBLOCKS][BLOCK_SIZE];
    using const_blocked_matrix_t = const float (&) [NBLOCKS][BLOCK_SIZE][NBLOCKS][BLOCK_SIZE];
    auto blockA = reinterpret_cast<const_blocked_matrix_t>(A[0][0]);
    auto blockB = reinterpret_cast<const_blocked_matrix_t>(B[0][0]);
    auto blockC = reinterpret_cast<blocked_matrix_t>(C[0][0]);
    for (int i = 0; i < MATRIX_SIZE; i++)
                                                  Multiply using pre-transposed matrix B
    for (int j = 0; j < MATRIX_SIZE; j++)
                                                    (which is treated as column-major)
        C[i][i] = 0.;
                                                        ... just like GEMM_Test_0_4
    for (int bi = 0; bi < NBLOCKS; bi++)
    for (int bj = 0; bj < NBLOCKS; bj++)
        for (int bk = 0; bk < NBLOCKS; bk++)
            for (int ii = 0; ii < BLOCK_SIZE; ii++)
            for (int jj = 0; jj < BLOCK_SIZE; jj++)
                for (int kk = 0; kk < BLOCK_SIZE; kk++)
                    blockC[bi][ii][bj][jj] += blockA[bi][ii][bk][kk] * blockB[bj][jj][bk][kk];
```

GEMM routine (MatMatMultiply.cpp)

DenseAlgebra/GEMM_Test_0_5

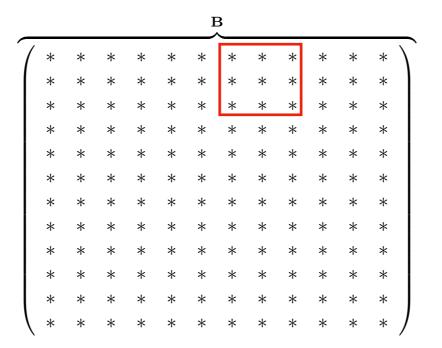
```
#include "MatMatMultiply.h"
[\ldots]
void MatMatTransposeMultiply(const float (&A)[MATRIX_SIZE][MATRIX_SIZE],
    const float (&B)[MATRIX_SIZE][MATRIX_SIZE], float (&C)[MATRIX_SIZE][MATRIX_SIZE])
    static constexpr int NBLOCKS = MATRIX_SIZE / BLOCK_SIZE;
    using blocked_matrix_t = float (&) [NBLOCKS][BLOCK_SIZE][NBLOCKS][BLOCK_SIZE];
    using const_blocked_matrix_t = const float (&) [NBLOCKS][BLOCK_SIZE][NBLOCKS][BLOCK_SIZE];
    auto blockA = reinterpret_cast<const_blocked_matrix_t>(A[0][0]);
    auto blockB = reinterpret_cast<const_blocked_matrix_t>(B[0][0]);
    auto blockC = reinterpret_cast<blocked_matrix_t>(C[0][0]);
    for (int i = 0; i < MATRIX_SIZE; i++)
                                                 Re-cast the input/output matrices so we
    for (int j = 0; j < MATRIX_SIZE; j++)
                                               can index them with blockID/subelementID
        C[i][i] = 0.;
                                                       ... just like GEMM_Test_0_2
    for (int bi = 0; bi < NBLOCKS; bi++)
    for (int bj = 0; bj < NBLOCKS; bj++)
        for (int bk = 0; bk < NBLOCKS; bk++)
            for (int ii = 0; ii < BLOCK_SIZE; ii++)
            for (int jj = 0; jj < BLOCK_SIZE; jj++)
                for (int kk = 0; kk < BLOCK_SIZE; kk++)
                    blockC[bi][ii][bj][jj] += blockA[bi][ii][bk][kk] * blockB[bj][jj][bk][kk];
```

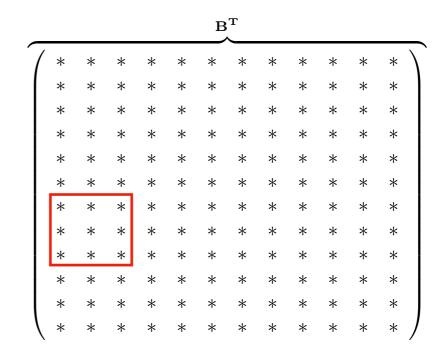
GEMM routine (MatMatMultiply.cpp) DenseAlgebra/GEMM_Test_0_5

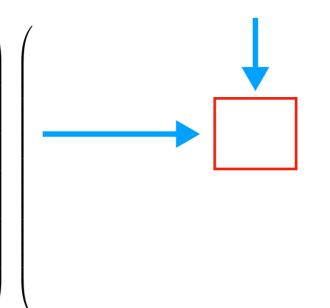
```
#include "MatMatMultiply.h"
[\ldots]
void MatMatTransposeMultiply(const float (&A)[MATRIX_SIZE][MATRIX_SIZE],
    const float (&B)[MATRIX_SIZE][MATRIX_SIZE], float (&C)[MATRIX_SIZE][MATRIX_SIZE])
    static constexpr int NBLOCKS = MATRIX_SIZE / BLOCK_SIZE;
    using blocked_matrix_t = float (&) [NBLOCKS][BLOCK_SIZE][NBLOCKS][BLOCK_SIZE];
    using const_blocked_matrix_t = const float (&) [NBLOCKS][BLOCK_SIZE][NBLOCKS][BLOCK_SIZE];
    auto blockA = reinterpret_cast<const_blocked_matrix_t>(A[0][0]);
    auto blockB = reinterpret_cast<const_blocked_matrix_t>(B[0][0]);
    auto blockC = reinterpret_cast<blocked_matrix_t>(C[0][0]);
    for (int i = 0; i < MATRIX_SIZE; i++)
                                                    Zero out the matrix C in the beginning
    for (int j = 0; j < MATRIX_SIZE; j++)
        C\Gamma i \Gamma \Gamma i \Gamma = 0.:
                                                 (easier to do, only N<sup>2</sup> operations/accesses)
    for (int bi = 0; bi < NBLOCKS; bi++)
    for (int bj = 0; bj < NBLOCKS; bj++)
        for (int bk = 0; bk < NBLOCKS; bk++)
            for (int ii = 0; ii < BLOCK_SIZE; ii++)
            for (int jj = 0; jj < BLOCK_SIZE; jj++)
                for (int kk = 0; kk < BLOCK_SIZE; kk++)
                    blockC[bi][ii][bj][jj] += blockA[bi][ii][bk][kk] * blockB[bj][jj][bk][kk];
```

GEMM routine (MatMatMultiply.cpp) | DenseAlgebra/GEMM_Test_0_5

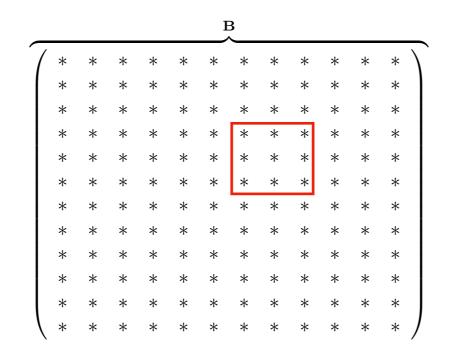
```
#include "MatMatMultiply.h"
[\ldots]
void MatMatTransposeMultiply(const float (&A)[MATRIX_SIZE][MATRIX_SIZE],
    const float (&B)[MATRIX_SIZE][MATRIX_SIZE], float (&C)[MATRIX_SIZE][MATRIX_SIZE])
    static constexpr int NBLOCKS = MATRIX_SIZE / BLOCK_SIZE;
    using blocked_matrix_t = float (&) [NBLOCKS][BLOCK_SIZE][NBLOCKS][BLOCK_SIZE];
    using const_blocked_matrix_t = const float (&) [NBLOCKS][BLOCK_SIZE][NBLOCKS][BLOCK_SIZE];
    auto blockA = reinterpret_cast<const_blocked_matrix_t>(A[0][0]);
    auto blockB = reinterpret_cast<const_blocked_matrix_t>(B[0][0]);
    auto blockC = reinterpret_cast<blocked_matrix_t>(C[0][0]);
    for (int i = 0; i < MATRIX_SIZE; i++)
    for (int j = 0; j < MATRIX_SIZE; j++)
        C[i][i] = 0.;
                                                  Iterate to do multiplication of blocks ...
    for (int bi = 0; bi < NBLOCKS; bi++)
    for (int bj = 0; bj < NBLOCKS; bj++)
        for (int bk = 0; bk < NBLOCKS; bk++)
            for (int ii = 0; ii < BLOCK_SIZE; ii++)
            for (int jj = 0; jj < BLOCK_SIZE; jj++)
                for (int kk = 0; kk < BLOCK_SIZE; kk++)
                    blockC[bi][ii][bj][jj] += blockA[bi][ii][bk][kk] * blockB[bj][jj][bk][kk];
```

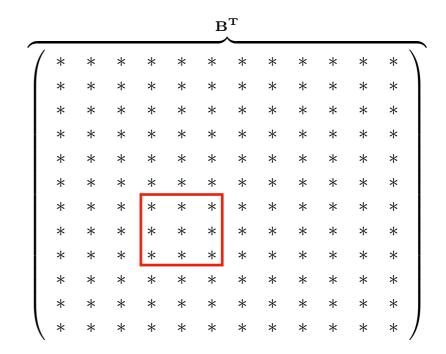


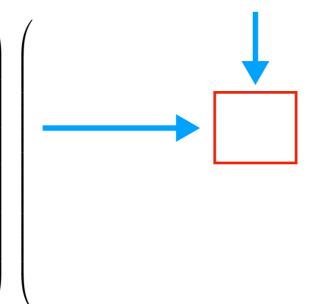




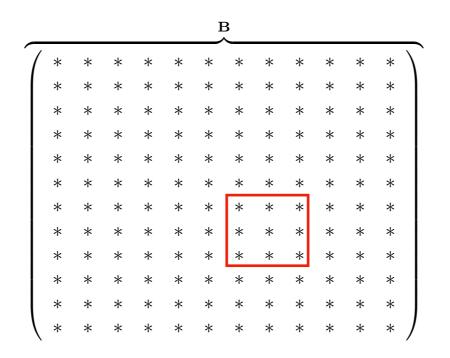
$$\begin{aligned} \text{for } i &= 1 \dots N \\ \text{for } j &= 1 \dots N \\ C_{ij} &\leftarrow 0 \\ \text{for } k &= 1 \dots N \\ C_{ij} &\leftarrow C_{ij} + A_{ik} [B^T]_{jk} \end{aligned}$$

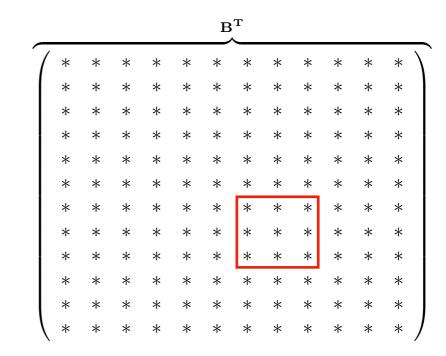


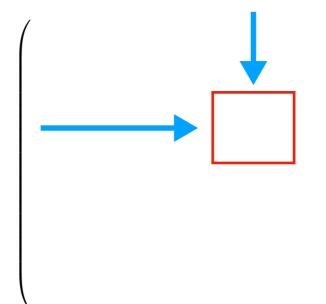




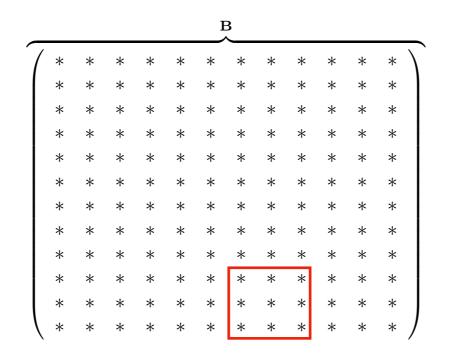
$$\begin{aligned} \text{for } i &= 1 \dots N \\ \text{for } j &= 1 \dots N \\ C_{ij} &\leftarrow 0 \\ \text{for } k &= 1 \dots N \\ C_{ij} &\leftarrow C_{ij} + A_{ik}[B^T]_{jk} \end{aligned}$$

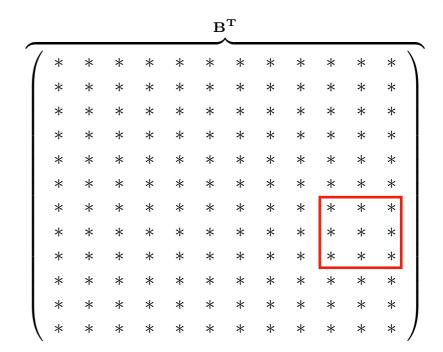


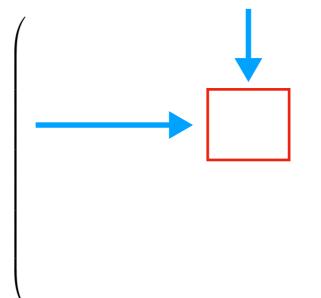




$$\begin{aligned} \text{for } i &= 1 \dots N \\ \text{for } j &= 1 \dots N \\ C_{ij} &\leftarrow 0 \\ \text{for } k &= 1 \dots N \\ C_{ij} &\leftarrow C_{ij} + A_{ik}[B^T]_{jk} \end{aligned}$$



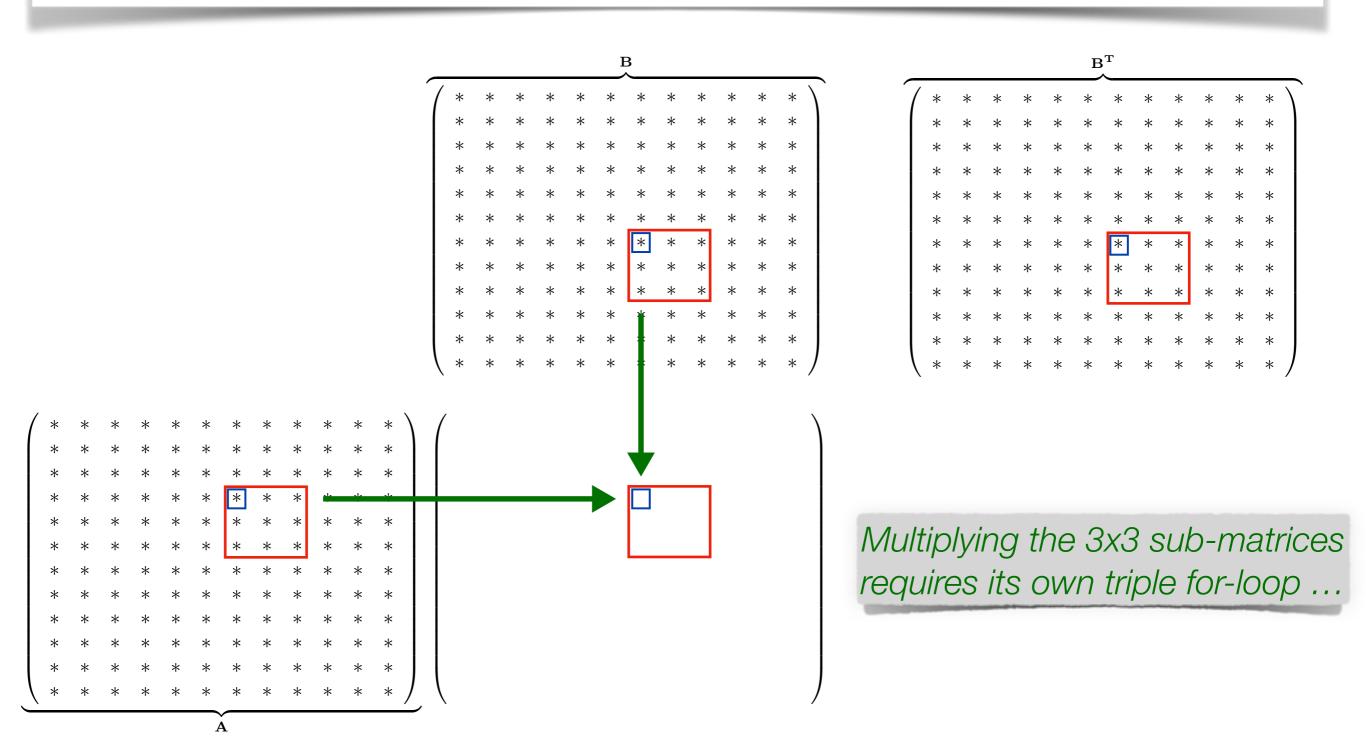


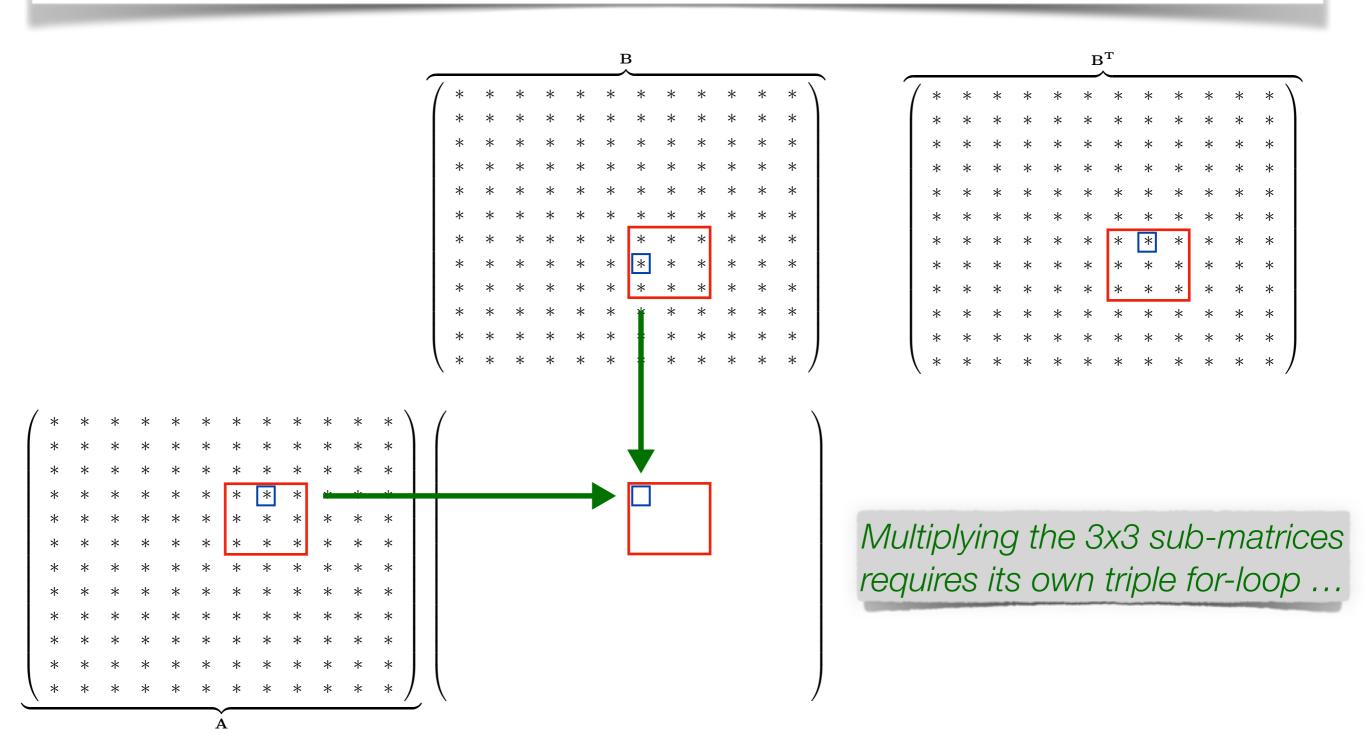


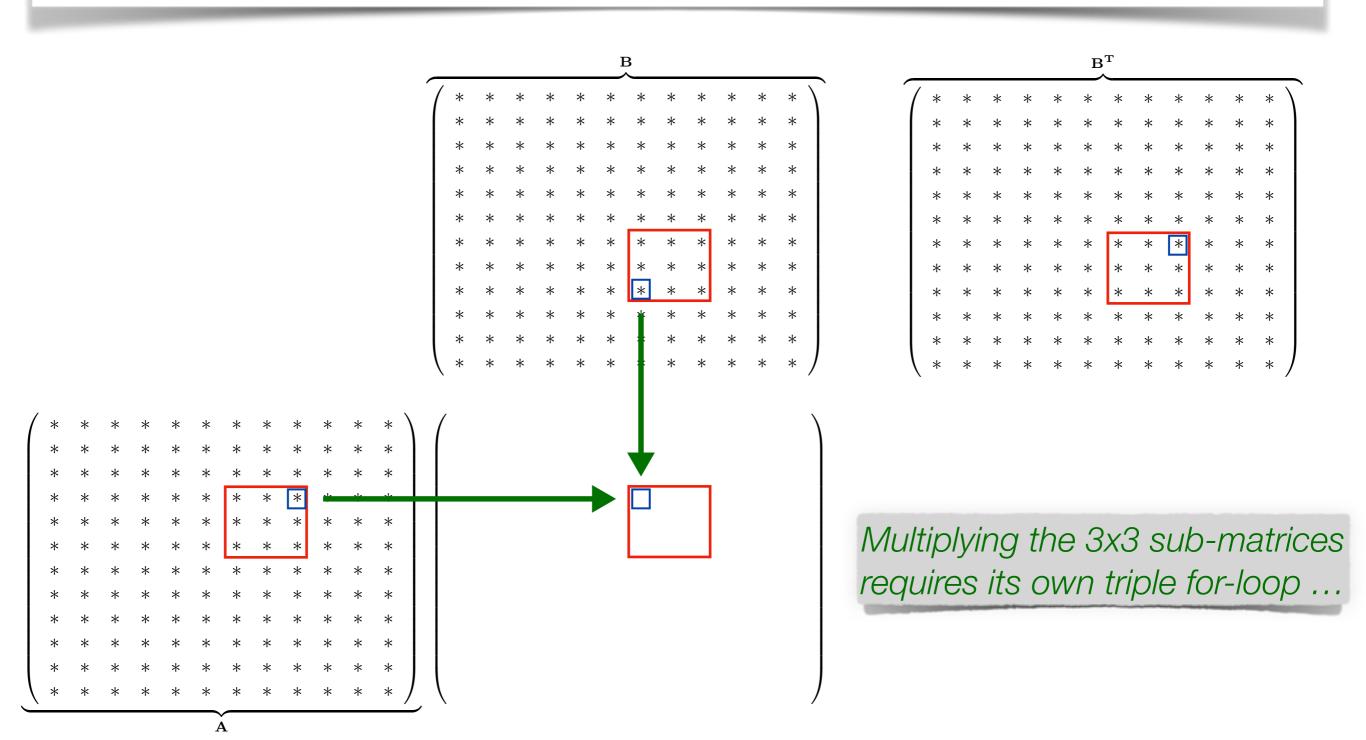
$$\begin{aligned} \text{for } i &= 1 \dots N \\ \text{for } j &= 1 \dots N \\ C_{ij} &\leftarrow 0 \\ \text{for } k &= 1 \dots N \\ C_{ij} &\leftarrow C_{ij} + A_{ik}[B^T]_{jk} \end{aligned}$$

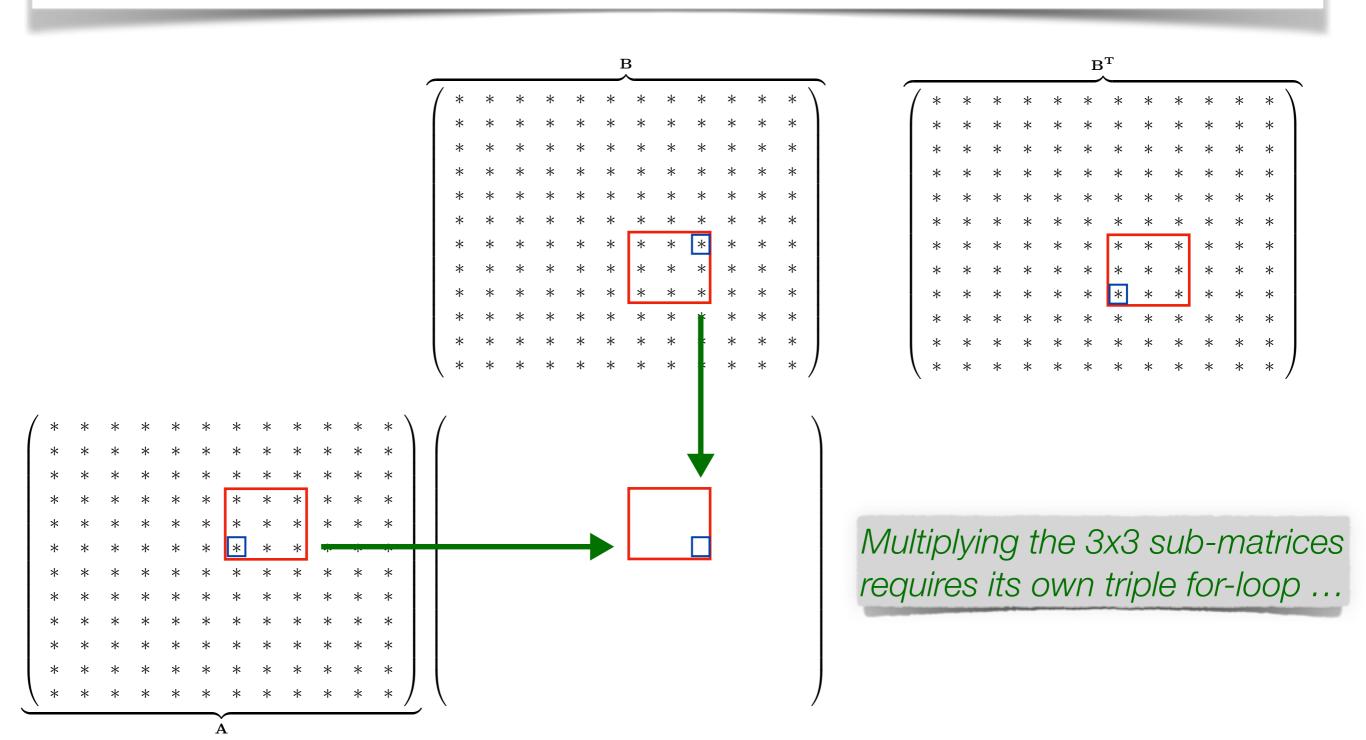
GEMM routine (MatMatMultiply.cpp) | DenseAlgebra/GEMM_Test_0_5

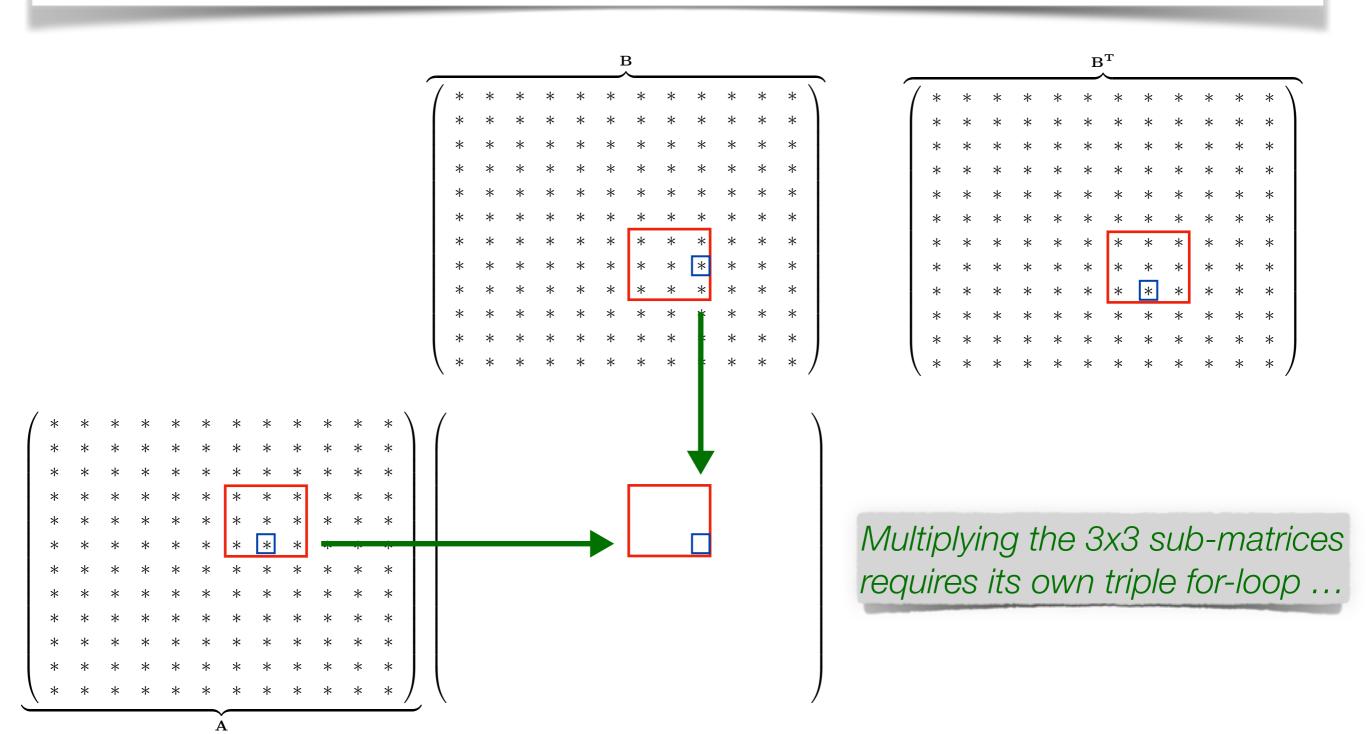
```
#include "MatMatMultiply.h"
[\ldots]
void MatMatTransposeMultiply(const float (&A)[MATRIX_SIZE][MATRIX_SIZE],
    const float (&B)[MATRIX_SIZE][MATRIX_SIZE], float (&C)[MATRIX_SIZE][MATRIX_SIZE])
    static constexpr int NBLOCKS = MATRIX_SIZE / BLOCK_SIZE;
    using blocked_matrix_t = float (&) [NBLOCKS][BLOCK_SIZE][NBLOCKS][BLOCK_SIZE];
    using const_blocked_matrix_t = const float (&) [NBLOCKS][BLOCK_SIZE][NBLOCKS][BLOCK_SIZE];
    auto blockA = reinterpret_cast<const_blocked_matrix_t>(A[0][0]);
    auto blockB = reinterpret_cast<const_blocked_matrix_t>(B[0][0]);
    auto blockC = reinterpret_cast<blocked_matrix_t>(C[0][0]);
    for (int i = 0; i < MATRIX_SIZE; i++)
    for (int j = 0; j < MATRIX_SIZE; j++)
        C[i][i] = 0.;
    for (int bi = 0; bi < NBLOCKS; bi++)
                                                      ... and iterate again within the blocks,
    for (int bj = 0; bj < NBLOCKS; bj++)
                                                              to multiply them together
        for (int bk = 0; bk < NBLOCKS; bk++)
            for (int ii = 0; ii < BLOCK_SIZE; ii++)</pre>
            for (int jj = 0; jj < BLOCK_SIZE; jj++)
                for (int kk = 0; kk < BLOCK_SIZE; kk++)
                    blockC[bi][ii][bj][jj] += blockA[bi][ii][bk][kk] * blockB[bj][jj][bk][kk];
```



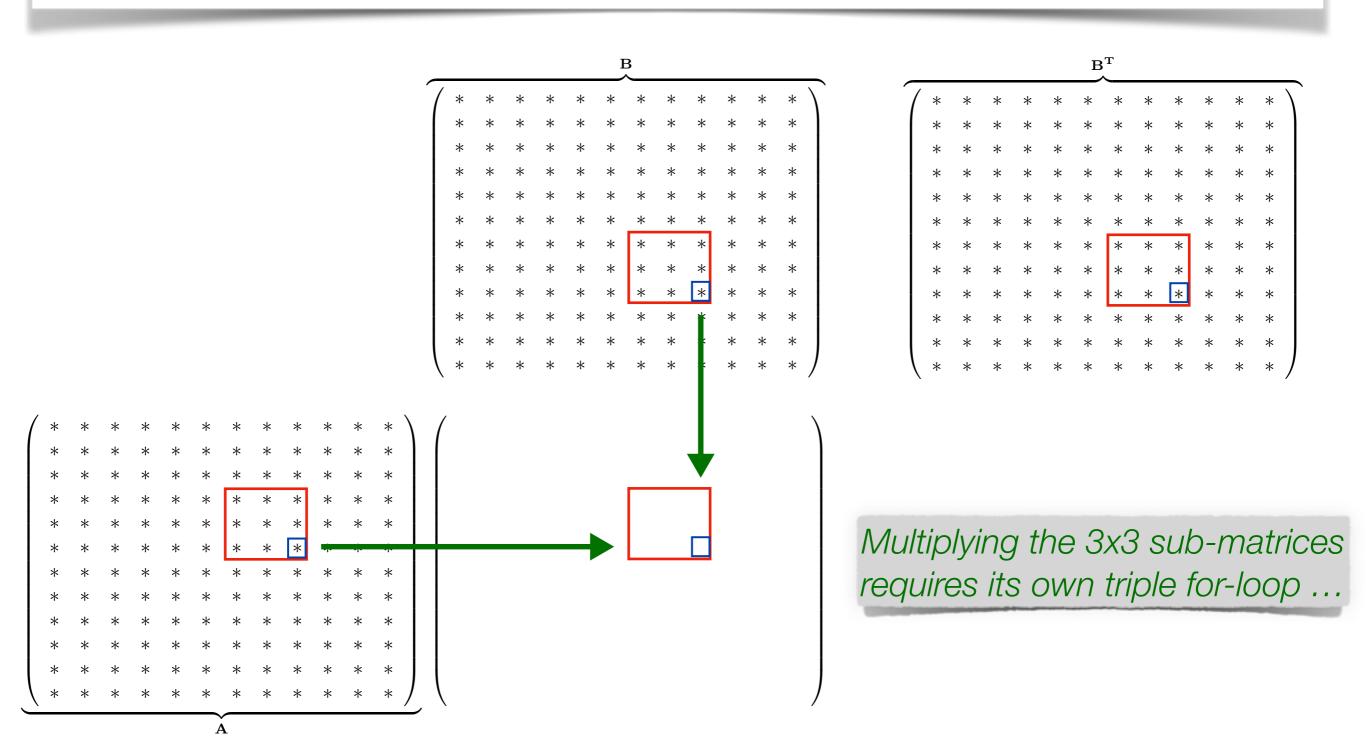








Combining blocking & pre-transposed B (or col-major B)



```
#include "MatMatMultiply.h"
[\ldots]
void MatMatTransposeMultiply(const float (&A)[MATRIX_SIZE][MATRIX_SIZE],
    const float (&B)[MATRIX_SIZE][MATRIX_SIZE], float (&C)[MATRIX_SIZE][MATRIX_SIZE])
    static constexpr int NBLOCKS = MATRIX_SIZE / BLOCK_SIZE;
    using blocked_matrix_t = float (&) [NBLOCKS][BLOCK_SIZE][NBLOCKS][BLOCK_SIZE];
    using const_blocked_matrix_t = const float (&) [NBLOCKS][BLOCK_SIZE][NBLOCKS][BLOCK_SIZE];
    auto blockA = reinterpret_cast<const_blocked_matrix_t>(A[0][0]);
    auto blockB = reinterpret_cast<const_blocked_matrix_t>(B[0][0]);
    auto blockC = reinterpret_cast<blocked_matrix_t>(C[0][0]);
    for (int i = 0; i < MATRIX_SIZE; i++)
    for (int j = 0; j < MATRIX_SIZE; j++)
        C[i][i] = 0.;
    for (int bi = 0; bi < NBLOCKS; bi++)
                                                      ... and iterate again within the blocks,
    for (int bj = 0; bj < NBLOCKS; bj++)
                                                              to multiply them together
        for (int bk = 0; bk < NBLOCKS; bk++)
            for (int ii = 0; ii < BLOCK_SIZE; ii++)</pre>
            for (int jj = 0; jj < BLOCK_SIZE; jj++)
                for (int kk = 0; kk < BLOCK_SIZE; kk++)
                    blockC[bi][ii][bj][jj] += blockA[bi][ii][bk][kk] * blockB[bj][jj][bk][kk];
```

```
#include "MatMatMultiply.h"
[\ldots]
void MatMatTransposeMultiply(const float (&A)[MATRIX_SIZE][MATRIX_SIZE],
    const float (&B)[MATRIX_SIZE][MATRIX_SIZE], float (&C)[MATRIX_SIZE][MATRIX_SIZE])
    static constexpr int NBLOCKS = MATRIX_SIZE / BLOCK_SIZE;
    using blocked_matrix_t = float (&) [NBLOCKS][BLOCK_SIZE][NBLOCKS][BLOCK_SIZE];
    using const_blocked_matrix_t = const float (&) [NBLOCKS][BLOCK_SIZE][NBLOCKS][BLOCK_SIZE];
    auto blockA = reinterpret_cast<const_blocked_matrix_t>(A[0][0]);
    auto blockB = reinterpret_cast<const_blocked_matrix_t>(B[0][0]);
    auto blockC = reinterpret_cast<blocked_matrix_t>(C[0][0]);
    for (int i = 0; i < MATRIX_SIZE; i++)
    for (int j = 0; j < MATRIX_SIZE; j++)
                                                            No parallelization yet!
        C[i][i] = 0.;
    for (int bi = 0; bi < NBLOCKS; bi++)
    for (int bj = 0; bj < NBLOCKS; bj++)
        for (int bk = 0; bk < NBLOCKS; bk++)
            for (int ii = 0; ii < BLOCK_SIZE; ii++)
            for (int jj = 0; jj < BLOCK_SIZE; jj++)
                for (int kk = 0; kk < BLOCK_SIZE; kk++)
                    blockC[bi][ii][bj][jj] += blockA[bi][ii][bk][kk] * blockB[bj][jj][bk][kk];
```

```
#include "MatMatMultiply.h"
[\ldots]
void MatMatTransposeMultiply(const float (&A)[MATRIX_SIZE][MATRIX_SIZE],
    const float (&B)[MATRIX_SIZE][MATRIX_SIZE], float (&C)[MATRIX_SIZE][MATRIX_SIZE])
    static constexpr int NBLOCKS = MATRIX_SIZE / BLOCK_SIZE;
    using blocked_matrix_t = float (&) [NBLOCKS][BLOCK_SIZE][NBLOCKS][BLOCK_SIZE];
    using const_blocked_matrix_t = const float (&) [NBLOCKS][BLOCK_SIZE][NBLOCKS][BLOCK_SIZE];
    auto blockA = reinterpret_cast<const_blocked_matrix_t>(A[0][0]);
                                                                      At matrix size = 1024
    auto blockB = reinterpret_cast<const_blocked_matrix_t>(B[0][0]);
    auto block( = raintarnest cast/blocked matrix + (([0][0]).
                                                   Execution:
    for (int i = 0Transposing second matrix factor ... [Elapsed time : 37.801ms]
    for (int j = 0 Running candidate kernel for correctness test ... [Elapsed time : 860.326ms]
        C[i][j] = Running reference kernel for correctness test ... [Elapsed time : 3.38718ms]
                  Discrepancy between two methods: 7.24792e-05
    for (int bi = Running kernel for performance run # 1 ... [Elapsed time : 765.428ms]
    for (int bj = Running kernel for performance run # 2 ... [Elapsed time : 686.641ms]
        for (int bRunning kernel for performance run # 3 ... [Elapsed time : 687.419ms]
            for (iRunning kernel for performance run # 4 ... [Elapsed time : 685.17ms]
            for (iRunning kernel for performance run # 5 ... [Elapsed time : 687.214ms]
                foRunning kernel for performance run # 6 ... [Elapsed time : 686.913ms]
                  Running kernel for performance run # 7 ... [Elapsed time : 685.123ms]
                  Running kernel for performance run # 8 ... [Elapsed time : 686.015ms]
                  [\ldots]
```

```
[...]
void MatMatTransposeMultiply(const float (&A)[MATRIX_SIZE][MATRIX_SIZE],
    const float (&B)[MATRIX_SIZE][MATRIX_SIZE], float (&C)[MATRIX_SIZE][MATRIX_SIZE])
    static constexpr int NBLOCKS = MATRIX_SIZE / BLOCK_SIZE;
    using blocked_matrix_t = float (&) [NBLOCKS][BLOCK_SIZE][NBLOCKS][BLOCK_SIZE];
    using const_blocked_matrix_t = const float (&) [NBLOCKS][BLOCK_SIZE][NBLOCKS][BLOCK_SIZE];
    auto blockA = reinterpret_cast<const_blocked_matrix_t>(A[0][0]);
    auto blockB = reinterpret_cast<const_blocked_matrix_t>(B[0][0]);
    auto blockC = reinterpret_cast<blocked_matrix_t>(C[0][0]);
#pragma omp parallel for
    for (int i = 0; i < MATRIX_SIZE; i++)
    for (int j = 0; j < MATRIX_SIZE; j++)
        C[i][j] = 0.;
#pragma omp parallel for
    for (int bi = 0; bi < NBLOCKS; bi++)
    for (int bj = 0; bj < NBLOCKS; bj++)
        for (int bk = 0; bk < NBLOCKS; bk++)
            for (int ii = 0; ii < BLOCK_SIZE; ii++)
            for (int jj = 0; jj < BLOCK_SIZE; jj++) {</pre>
                float partial_result = 0.; // Needed by some compilers for correctness
#pragma omp simd reduction (+:partial_result)
                for (int kk = 0; kk < BLOCK_SIZE; kk++)
                    partial_result += blockA[bi][ii][bk][kk] * blockB[bj][jj][bk][kk];
                blockC[bi][ii][bj][jj] += partial_result;
```

```
[...]
void MatMatTransposeMultiply(const float (&A)[MATRIX_SIZE][MATRIX_SIZE],
    const float (&B)[MATRIX_SIZE][MATRIX_SIZE], float (&C)[MATRIX_SIZE][MATRIX_SIZE])
    static constexpr int NBLOCKS = MATRIX_SIZE / BLOCK_SIZE;
    using blocked_matrix_t = float (&) [NBLOCKS][BLOCK_SIZE][NBLOCKS][BLOCK_SIZE];
    using const_blocked_matrix_t = const float (&) [NBLOCKS][BLOCK_SIZE][NBLOCKS][BLOCK_SIZE];
    auto blockA = reinterpret_cast<const_blocked_matrix_t>(A[0][0]);
    auto blockB = reinterpret_cast<const_blocked_matrix_t>(B[0][0]);
    auto blockC = reinterpret_cast<blocked_matrix_t>(C[0][0]);
#pragma omp parallel for
    for (int i = 0; i < MATRIX_SIZE; i++)
    for (int j = 0; j < MATRIX_SIZE; j++)
        C[i][j] = 0.;
                                                    Use multithreading across rows of A
#pragma omp parallel for
                                                           (or rows of blocks of A)
    for (int bi = 0; bi < NBLOCKS; bi++)
    for (int bj = 0; bj < NBLOCKS; bj++)
        for (int bk = 0; bk < NBLOCKS; bk++)
            for (int ii = 0; ii < BLOCK_SIZE; ii++)
            for (int jj = 0; jj < BLOCK_SIZE; jj++) {</pre>
                float partial_result = 0.; // Needed by some compilers for correctness
#pragma omp simd reduction (+:partial_result)
                for (int kk = 0; kk < BLOCK_SIZE; kk++)
                    partial_result += blockA[bi][ii][bk][kk] * blockB[bj][jj][bk][kk];
                blockC[bi][ii][bj][jj] += partial_result;
```

```
[...]
void MatMatTransposeMultiply(const float (&A)[MATRIX_SIZE][MATRIX_SIZE],
    const float (&B)[MATRIX_SIZE][MATRIX_SIZE], float (&C)[MATRIX_SIZE][MATRIX_SIZE])
    static constexpr int NBLOCKS = MATRIX_SIZE / BLOCK_SIZE;
    using blocked_matrix_t = float (&) [NBLOCKS][BLOCK_SIZE][NBLOCKS][BLOCK_SIZE];
    using const_blocked_matrix_t = const float (&) [NBLOCKS][BLOCK_SIZE][NBLOCKS][BLOCK_SIZE];
    auto blockA = reinterpret_cast<const_blocked_matrix_t>(A[0][0]);
    auto blockB = reinterpret_cast<const_blocked_matrix_t>(B[0][0]);
    auto blockC = reinterpret_cast<blocked_matrix_t>(C[0][0]);
#pragma omp parallel for
    for (int i = 0; i < MATRIX_SIZE; i++)
    for (int j = 0; j < MATRIX_SIZE; j++)
        C[i][j] = 0.;
                                               Use SIMD to accelerate the "dot-product-like"
#pragma omp parallel for
                                                     reduction in matrix-matrix multiply
    for (int bi = 0; bi < NBLOCKS; bi++)
    for (int bj = 0; bj < NBLOCKS; bj++)
        for (int bk = 0; bk < NBLOCKS; bk++)
            for (int ii = 0; ii < BLOCK_SIZE; ii++)
            for (int jj = 0; jj < BLOCK_SIZE; jj++) {</pre>
                float partial_result = 0.; // Needed by some compilers for correctness
#pragma omp simd reduction (+:partial_result)
                for (int kk = 0; kk < BLOCK_SIZE; kk++)
                    partial_result += blockA[bi][ii][bk][kk] * blockB[bj][jj][bk][kk];
                blockC[bi][ii][bj][jj] += partial_result;
```

```
[...]
void MatMatTransposeMultiply(const float (&A)[MATRIX_SIZE][MATRIX_SIZE],
    const float (&B)[MATRIX_SIZE][MATRIX_SIZE], float (&C)[MATRIX_SIZE][MATRIX_SIZE])
{
    static constexpr int NBLOCKS = MATRIX_SIZE / BLOCK_SIZE;
    using blocked_matrix_t = float (&) [NBLOCKS][BLOCK_SIZE][NBLOCKS][BLOCK_SIZE];
    using const_blocked_matrix_t = const float (&) [NBLOCKS][BLOCK_SIZE][NBLOCKS][BLOCK_SIZE];
    auto blockA = reinterpret_cast<const_blocked_matrix_t>(A[0][0]);
    auto blockB = reinterpret_cast<const_blocked_matrix_t>(B[0][0]);
    auto blockC = reinterpret_cast<blocked_matrix_t>(C[0][0]);
#pragma omp parallel for
    for (int i = 0; i < MATRIX_SIZE; i++)
    for (int j = 0; j < MATRIX_SIZE; j++)
                                                  Note: It should have been sufficient
        C[i][j] = 0.;
                                                            to write it like this:
#pragma omp parallel for
                                          (and this does work correctly in most compilers ...)
    for (int bi = 0; bi < NBLOCKS; bi++)
    for (int bj = 0; bj < NBLOCKS; bj++)
        for (int bk = 0; bk < NBLOCKS; bk++)
            for (int ii = 0; ii < BLOCK_SIZE; ii++)</pre>
            for (int jj = 0; jj < BLOCK_SIZE; jj++)
#pragma omp simd
                for (int kk = 0; kk < BLOCK_SIZE; kk++)
                    blockC[bi][ii][bj][jj] += blockA[bi][ii][bk][kk] * blockB[bj][jj][bk][kk];
```

```
[...]
void MatMatTransposeMultiply(const float (&A)[MATRIX_SIZE][MATRIX_SIZE],
    const float (&B)[MATRIX_SIZE][MATRIX_SIZE], float (&C)[MATRIX_SIZE][MATRIX_SIZE])
{
    static constexpr int NBLOCKS = MATRIX_SIZE / BLOCK_SIZE;
    using blocked_matrix_t = float (&) [NBLOCKS][BLOCK_SIZE][NBLOCKS][BLOCK_SIZE];
    using const_blocked_matrix_t = const float (&) [NBLOCKS][BLOCK_SIZE][NBLOCKS][BLOCK_SIZE];
    auto blockA = reinterpret_cast<const_blocked_matrix_t>(A[0][0]);
    auto blockB = reinterpret_cast<const_blocked_matrix_t>(B[0][0]);
    auto blockC = reinterpret_cast<blocked_matrix_t>(C[0][0]);
#pragma omp parallel for
    for (int i = 0; i < MATRIX_SIZE; i++)
    for (int j = 0; j < MATRIX_SIZE; j++)
        C[i][j] = 0.;
                                               Note the pattern that suggests SIMD ...
#pragma omp parallel for
    for (int bi = 0; bi < NBLOCKS; bi++)
    for (int bj = 0; bj < NBLOCKS; bj++)
        for (int bk = 0; bk < NBLOCKS; bk++)
            for (int ii = 0; ii < BLOCK_SIZE; ii++)
            for (int jj = 0; jj < BLOCK_SIZE; jj++)
#pragma omp simd
                for (int kk = 0; kk < BLOCK_SIZE; kk++)
                    blockC[bi][ii][bj][jj] += blockA[bi][ii][bk][kk] * blockB[bj][jj][bk][kk];
```

```
[...]
void MatMatTransposeMultiply(const float (&A)[MATRIX_SIZE][MATRIX_SIZE],
    const float (&B)[MATRIX_SIZE][MATRIX_SIZE], float (&C)[MATRIX_SIZE][MATRIX_SIZE])
    static constexpr int NBLOCKS = MATRIX_SIZE / BLOCK_SIZE;
    using blocked_matrix_t = float (&) [NBLOCKS][BLOCK_SIZE][NBLOCKS][BLOCK_SIZE];
    using const_blocked_matrix_t = const float (&) [NBLOCKS][BLOCK_SIZE][NBLOCKS][BLOCK_SIZE];
    auto blockA = reinterpret_cast<const_blocked_matrix_t>(A[0][0]);
    auto blockB = reinterpret_cast<const_blocked_matrix_t>(B[0][0]);
    auto blockC = reinterpret_cast<blocked_matrix_t>(C[0][0]);
#pragma omp parallel for
    for (int i = 0; i < MATRIX_SIZE; i++)
    for (int j = 0; j < MATRIX_SIZE; j++)
        C[i][j] = 0.;
                                          ... but some versions of gcc/g++ seem to engage
                                            in unsafe optimizations (leading to errors) if you
#pragma omp parallel for
    for (int bi = 0; bi < NBLOCKS; bi++)
                                            don't use an intermediate variable for reduction
    for (int bj = 0; bj < NBLOCKS; bj++)
        for (int bk = 0; bk < NBLOCKS; bk++)
            for (int ii = 0; ii < BLOCK_SIZE; ii++)
            for (int jj = 0; jj < BLOCK_SIZE; jj++) {</pre>
                float partial_result = 0.; // Needed by some compilers for correctness
#pragma omp simd reduction (+:partial_result)
                for (int kk = 0; kk < BLOCK_SIZE; kk++)
                    partial_result += blockA[bi][ii][bk][kk] * blockB[bj][jj][bk][kk];
                blockC[bi][ii][bj][jj] += partial_result;
```

```
[...]
void MatMatTransposeMultiply(const float (&A)[MATRIX_SIZE][MATRIX_SIZE],
    const float (&B)[MATRIX_SIZE][MATRIX_SIZE], float (&C)[MATRIX_SIZE][MATRIX_SIZE])
    static constexpr int NBLOCKS = MATRIX_SIZE / BLOCK_SIZE;
    using blocked_matrix_t = float (&) [NBLOCKS][BLOCK_SIZE][NBLOCKS][BLOCK_SIZE];
    using const_blocked_matrix_t = const float (&) [NBLOCKS][BLOCK_SIZE][NBLOCKS][BLOCK_SIZE];
    auto blockA = reinterpret_cast<const_blocked_matrix_t>(A[0][0]);
    auto blockB = reinterpret_cast<const_blocked_matrix_t>(B[0][0]);
    auto blockC = reinterpret_cast<blocked_matrix_t>(C[0][0]);
#pragma omp parallel for
                                                      Matrix size 1024 x 1024
    for (int i = 0; i < MATRIX_SIZE; i++)
    for (int j = 0; j < MATRIX_SIZE; j++)
        C[i][j] = \rho
                                                   Execution:
#pragma omp parallTransposing second matrix factor ... [Elapsed time : 39.6778ms]
    for (int bi = Running candidate kernel for correctness test ... [Elapsed time : 23.9182ms]
    for (int bj = Running reference kernel for correctness test ... [Elapsed time : 2.6098ms]
        for (int bDiscrepancy between two methods: 3.8147e-05
            for (iRunning kernel for performance run # 1 ... [Elapsed time : 14.682ms]
            for (iRunning kernel for performance run # 2 ... [Elapsed time : 14.4771ms]
                fl Running kernel for performance run # 3 ... [Elapsed time : 14.4331ms]
#pragma omp simd rRunning kernel for performance run # 4 ... [Elapsed time : 14.7571ms]
                foRunning kernel for performance run # 5 ... [Elapsed time : 14.6737ms]
                  Running kernel for performance run # 6 ... [Elapsed time : 14.5883ms]
                bl Running kernel for performance run # 7 ... [Elapsed time : 14.6881ms]
                  Running kernel for performance run # 8 ... [Elapsed time : 13.9368ms]
                  [\ldots]
```

```
[...]
void MatMatTransposeMultiply(const float (&A)[MATRIX_SIZE][MATRIX_SIZE],
    const float (&B)[MATRIX_SIZE][MATRIX_SIZE], float (&C)[MATRIX_SIZE][MATRIX_SIZE])
    static constexpr int NBLOCKS = MATRIX_SIZE / BLOCK_SIZE;
    using blocked_matrix_t = float (&) [NBLOCKS][BLOCK_SIZE][NBLOCKS][BLOCK_SIZE];
    using const_blocked_matrix_t = const float (&) [NBLOCKS][BLOCK_SIZE][NBLOCKS][BLOCK_SIZE];
    auto blockA = reinterpret_cast<const_blocked_matrix_t>(A[0][0]);
    auto blockB = reinterpret_cast<const_blocked_matrix_t>(B[0][0]);
    auto blockC = reinterpret_cast<blocked_matrix_t>(C[0][0]);
#pragma omp parallel for
    for (int i = 0; i < MATRIX_SIZE; i++)
                                                      Matrix size 2048 x 2048
    for (int j = 0; j < MATRIX_SIZE; j++)
        C[i][j] = \rho
                                                   Execution:
#pragma omp parallTransposing second matrix factor ... [Elapsed time : 40.4148ms]
    for (int bi = Running candidate kernel for correctness test ... [Elapsed time : 116.462ms]
    for (int bj = Running reference kernel for correctness test ... [Elapsed time : 16.2658ms]
        for (int bDiscrepancy between two methods: 4.57764e-05
            for (iRunning kernel for performance run # 1 ... [Elapsed time : 105.37ms]
            for (iRunning kernel for performance run # 2 ... [Elapsed time : 104.903ms]
                fl Running kernel for performance run # 3 ... [Elapsed time : 104.987ms]
#pragma omp simd rRunning kernel for performance run # 4 ... [Elapsed time : 108.066ms]
                foRunning kernel for performance run # 5 ... [Elapsed time : 110.45ms]
                  Running kernel for performance run # 6 ... [Elapsed time : 111.708ms]
                bl Running kernel for performance run # 7 ... [Elapsed time : 110.166ms]
                  Running kernel for performance run # 8 ... [Elapsed time : 109.819ms]
                  [...]
```

```
#include "MatMatMultiply.h"
#include "mkl.h"
void MatMatMultiply(const float (&A)[MATRIX_SIZE][MATRIX_SIZE],
    const float (&B)[MATRIX_SIZE][MATRIX_SIZE], float (&C)[MATRIX_SIZE][MATRIX_SIZE])
    cblas_sgemm(
        CblasRowMajor,
        CblasNoTrans,
        CblasNoTrans,
        MATRIX_SIZE,
        MATRIX_SIZE,
        MATRIX_SIZE,
        1.,
        A[0][0]
        MATRIX_SIZE,
        &B[0][0],
        MATRIX_SIZE,
        0.,
        &C[0][0],
       MATRIX_SIZE
```

);

(compare with MKL) At matrix size = 2048

Execution:

```
Running test iteration 1 [Elapsed time : 61.1167ms]
Running test iteration 2 [Elapsed time: 14.2691ms]
Running test iteration 3 [Elapsed time: 14.1298ms]
Running test iteration 4 [Elapsed time: 14.2985ms]
Running test iteration 5 [Elapsed time: 14.2199ms]
Running test iteration 6 [Elapsed time: 14.0035ms]
Running test iteration 7 [Elapsed time: 14.2607ms]
Running test iteration 8 [Elapsed time: 14.0081ms]
Running test iteration 9 [Elapsed time: 15.484ms]
Running test iteration 10 [Elapsed time: 12.076ms]
```