Blue Waters Petascale Semester Curriculum v1.0

Unit 9: Optimization

Lesson 1: Cache Efficient Matrix Multiplication

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for the Shodor Education Foundation, Inc.

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Effective Caching for Matrix Multiplication

Cache Memory

- An important part of the memory hierarchy in any computer system
- Utilizes different technology compared to RAM
  - Faster
  - Uses more power
  - Costs more
- Gives the illusion of a large (RAM size), fast (cache speed) memory
- Compromise between cost, access time and size
- Program execution depends on efficiently utilizing the cache

Matrix Multiplication

- Matrices and matrix multiplication are very common in a variety of Engineering and Scientific Computing problems
- An n X n matrix A is mathematically written as:

$$A = \begin{bmatrix} a_{0,0} & a_{0,1} & \cdots & a_{0,n-1} \\ a_{1,0} & a_{1,1} & \cdots & a_{1,n-1} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n-1,0} & a_{n-1,1} & \cdots & a_{n-1,n-1} \end{bmatrix}$$

- Matrix multiplication is mathematically written as:

$$C = AB$$

- Where A, B and C are all n X n matrices

Matrix Multiplication

- Each element in C requires n multiplications and $n - 1$ additions
- Each element in C is computed by multiplying a row of matrix A with a column of matrix B, for example,

$$\begin{bmatrix} c_{0,0} & c_{0,1} & \cdots & c_{0,n-1} \\ \boxed{c_{1,0}} & c_{1,1} & \cdots & c_{1,n-1} \\ \vdots & \vdots & \ddots & \vdots \\ c_{n-1,0} & c_{n-1,1} & \cdots & c_{n-1,n-1} \end{bmatrix} = \begin{bmatrix} a_{0,0} & a_{0,1} & \cdots & a_{0,n-1} \\ a_{1,0} & a_{1,1} & \cdots & a_{1,n-1} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n-1,0} & a_{n-1,1} & \cdots & a_{n-1,n-1} \end{bmatrix} * \begin{bmatrix} b_{0,0} & b_{0,1} & \cdots & b_{0,n-1} \\ b_{1,0} & b_{1,1} & \cdots & b_{1,n-1} \\ \vdots & \vdots & \ddots & \vdots \\ b_{n-1,0} & b_{n-1,1} & \cdots & b_{n-1,n-1} \end{bmatrix}$$

- $c_{1,0}$ is the sum of the products of the elements of row 1 of matrix A and column 0 of matrix B
- Or more generally,

$$c_{i,j} = \sum_{k=0}^{n-1} a_{i,k} b_{k,j}$$

Matrix Memory Access

- The main memory of a computer system can be thought of as a long linear array, where elements are stored at consecutive memory locations
- A matrix is stored in memory either by rows (row major order) or columns (column major order)
- The **C** language uses row major order, while Fortran uses column major order
- A matrix in **C** is stored as:

Row 0	Row 1	. . .	Row n - 1

- Optimal cache utilization occurs when sequential memory elements are accessed
  - For the matrix multiplication example above, matrix *A* is efficiently accessed but matrix *B* is not

Matrix Multiplication Transpose

- Element access to matrix B can be made cache efficient by storing matrix B in column major order
- This is the same as computing the ***transpose*** of B
- In this case, the elements of the rows of matrix A are multiplied by the elements of the rows of matrix B

$$\begin{bmatrix} c_{0,0} & c_{0,1} & \cdots & c_{0,n-1} \\ \boxed{c_{1,0}} & c_{1,1} & \cdots & c_{1,n-1} \\ \vdots & \vdots & \ddots & \vdots \\ c_{n-1,0} & c_{n-1,1} & \cdots & c_{n-1,n-1} \end{bmatrix} = \begin{bmatrix} a_{0,0} & a_{0,1} & \cdots & a_{0,n-1} \\ a_{1,0} & a_{1,1} & \cdots & a_{1,n-1} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n-1,0} & a_{n-1,1} & \cdots & a_{n-1,n-1} \end{bmatrix} * \begin{bmatrix} b_{0,0} & b_{1,0} & \cdots & b_{n-1,0} \\ b_{0,1} & b_{1,1} & \cdots & b_{n-1,0} \\ \vdots & \vdots & \ddots & \vdots \\ b_{0,n-1} & b_{1,n-1} & \cdots & b_{n-1,n-1} \end{bmatrix}$$

$$c_{i,j} = \sum_{k=0}^{n-1} a_{i,k} b_{j,k}$$

Matrix Multiplication

- Matrix multiplication using the transpose of the B matrix more efficiently utilizes the cache
- Both matrix multiplication techniques inefficiently use the cache because the data must be brought into the cache multiple times
  - Each row of matrix A is multiplied by each row of matrix B
  - When the matrices are large, the rows of matrix B will need to be brought into the cache for each row in matrix A

Block Matrix Multiplication

- A better way of utilizing the cache is to perform block matrix multiplication, where the matrices are broken into blocks or tiles
- For example, a 4 X 4 matrix A can be made of 2 X 2 blocks or tiles each of size 2 X 2

$$A = \begin{bmatrix} a_{0,0} & a_{0,1} & a_{0,2} & a_{0,3} \\ a_{1,0} & a_{1,1} & a_{1,2} & a_{1,3} \\ a_{2,0} & a_{2,1} & a_{2,2} & a_{2,3} \\ a_{3,0} & a_{3,1} & a_{3,2} & a_{3,3} \end{bmatrix} = \begin{bmatrix} \begin{bmatrix} a_{0,0} & a_{0,1} \\ a_{1,0} & a_{1,1} \end{bmatrix} & \begin{bmatrix} a_{0,2} & a_{0,3} \\ a_{1,2} & a_{1,3} \end{bmatrix} \\ \begin{bmatrix} a_{2,0} & a_{2,1} \\ a_{3,0} & a_{3,1} \end{bmatrix} & \begin{bmatrix} a_{2,2} & a_{2,3} \\ a_{3,2} & a_{3,3} \end{bmatrix} \end{bmatrix} = \begin{bmatrix} A_{0,0} & A_{0,1} \\ A_{1,0} & A_{1,1} \end{bmatrix}$$

- Block matrix multiplications is

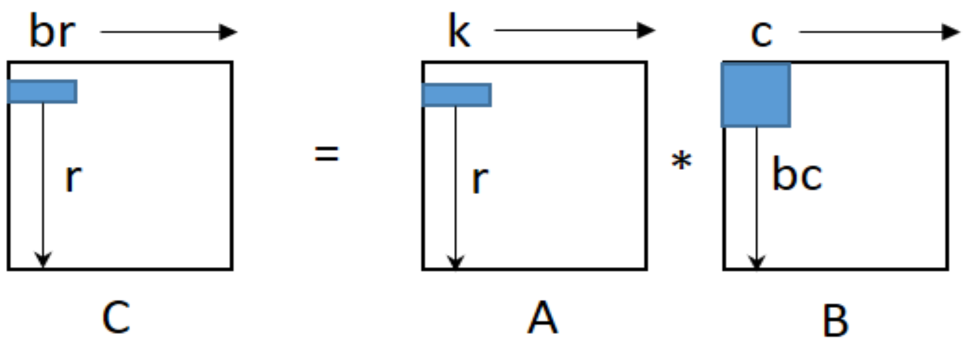
$$\begin{bmatrix} C_{0,0} & C_{0,1} \\ C_{1,0} & C_{1,1} \end{bmatrix} = \begin{bmatrix} A_{0,0} & A_{0,1} \\ A_{1,0} & A_{1,1} \end{bmatrix} \begin{bmatrix} B_{0,0} & B_{0,1} \\ B_{1,0} & B_{1,1} \end{bmatrix}$$

Block Matrix Multiplication

- The product matrix

$$C_{0,0} = A_{0,0}B_{0,0} + A_{0,1}B_{1,0}$$
$$C_{0,1} = A_{0,0}B_{0,1} + A_{0,1}B_{1,1}$$
$$C_{1,0} = A_{1,0}B_{0,0} + A_{1,1}B_{1,0}$$
$$C_{1,1} = A_{1,0}B_{0,1} + A_{1,1}B_{1,1}$$

- This technique efficiently utilizes the cache because all the elements in a block in matrix B are completely used for all computations and are not needed again

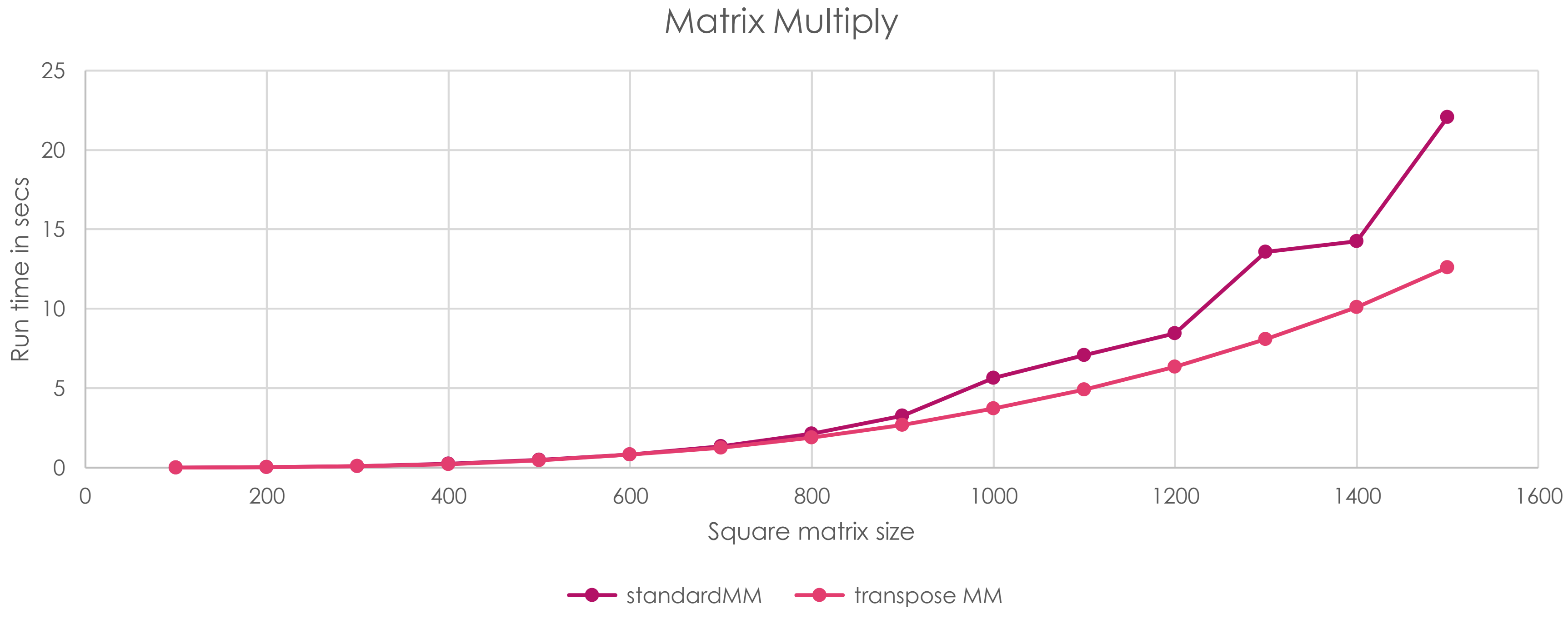


Matrix Multiply Program

- Two programs were written to time the standard matrix multiplication with both the transpose and the block matrix techniques
- Command line arguments are used to determine the size of the matrices
- All matrices utilize double-precision floating-point numbers
- Computational results are compared to ensure the product matrix is correctly determined

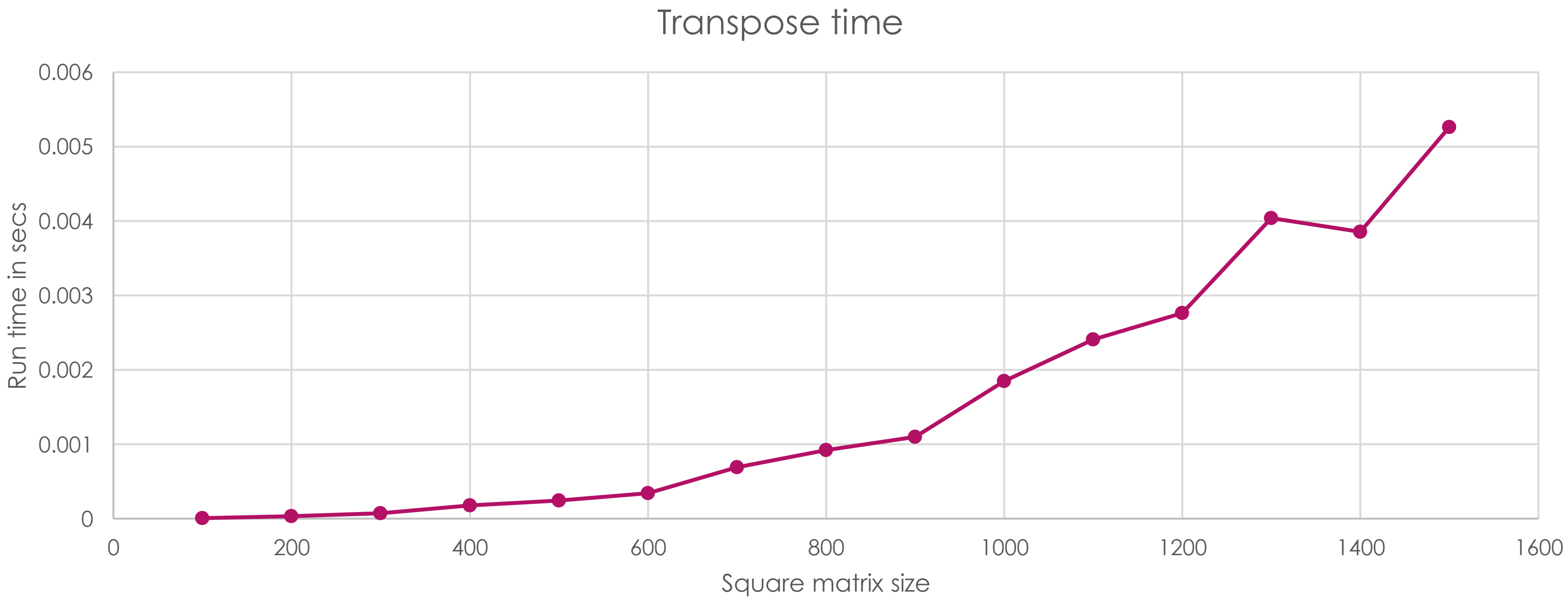
Program Results

- Timing results for standard matrix multiplication compared to transpose matrix multiplication



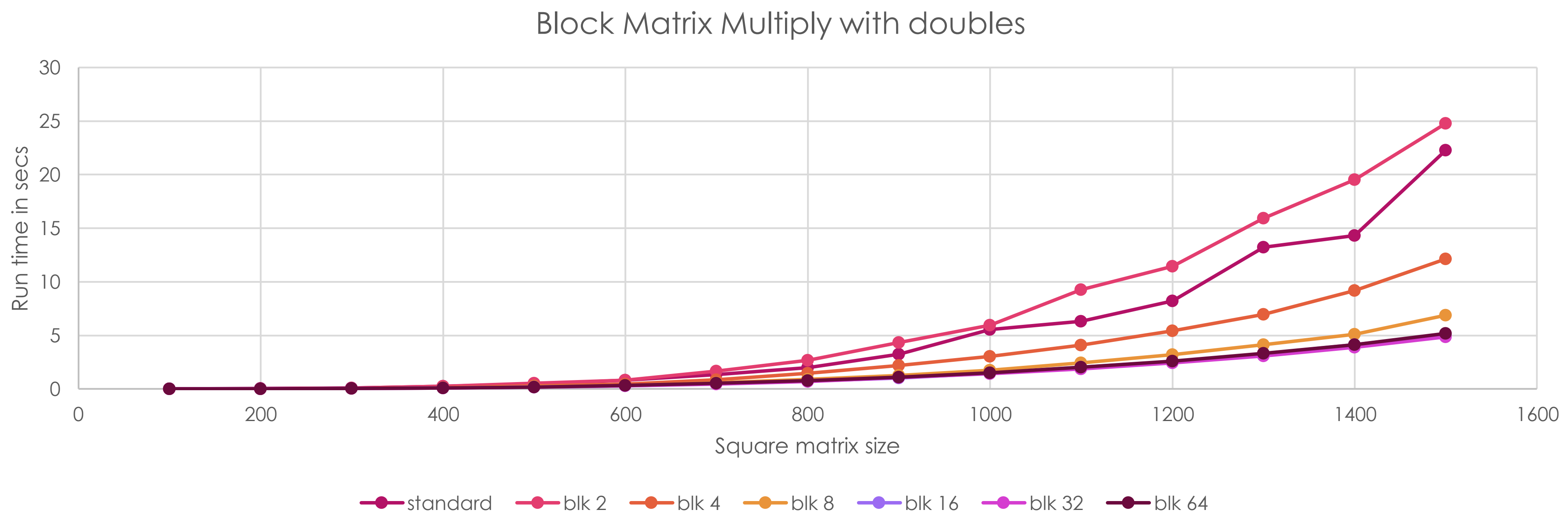
Program Results

- The time to transpose the matrix is negligible



Program Results

- The time to perform block matrix multiplication depends on the size of the block
- Blocks of size 8 X 8 or 16 X 16 appear to give the best performance



Program Results

- Block matrix multiply with blocks of size 16 X 16 appear to give the best performance