Data Parallelism and Matrix Multiplication

1. Data Parallelism
   - matrix-matrix multiplication
   - CUDA program structure

2. Code for Matrix-Matrix Multiplication
   - linear address system for 2-dimensional array
   - defining the kernel
   - the main program

3. Two Dimensional Arrays of Threads
   - using threadIdx.x and threadIdx.y

4. Examining Performance
   - counting flops

MCS 572 Lecture 31
Introduction to Supercomputing
Jan Verschelde, 2 November 2016
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Many applications process large amounts of data. Data parallelism refers to the property where many arithmetic operations can be safely performed on the data simultaneously. Consider the multiplication of matrices $A$ and $B$: $C = A \cdot B$, with

$$A = [a_{i,j}] \in \mathbb{R}^{n \times m}, \quad B = [b_{i,j}] \in \mathbb{R}^{m \times p}, \quad C = [c_{i,j}] \in \mathbb{R}^{n \times p}.$$ 

$c_{i,j}$ is the inner product of the $i$th row of $A$ with the $j$th column of $B$:

$$c_{i,j} = \sum_{k=1}^{m} a_{i,k} \cdot b_{k,j}.$$ 

All $c_{i,j}$’s can be computed independently from each other. For $n = m = p = 1,000$ we have 1,000,000 inner products.
Data parallelism in matrix multiplication

\[ c_{i,j} = \sum_{k=1}^{m} a_{i,k} \cdot b_{k,j} \]

**Introduction to Supercomputing (MCS 572)

Data Parallelism & Matrix Multiplication

L-31 2 November 2016 4 / 32
matrix-matrix multiplication on a GPU

Code for a device (the GPU) is defined in functions using the keyword `__global__` before the function definition.

Data parallel functions are called *kernels*.

Kernel functions generate a large number of threads.

In matrix-matrix multiplication, the computation can be implemented as a kernel where each thread computes one element in the result matrix.

To multiply two 1,000-by-1,000 matrices, the kernel using one thread to compute one element generates 1,000,000 threads when invoked.

CUDA threads are much lighter weight than CPU threads: they take very few cycles to generate and schedule thanks to efficient hardware support whereas CPU threads may require thousands of cycles.
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CUDA program structure

A CUDA program consists of several phases, executed on
- the host: if no data parallelism,
- the device: for data parallel algorithms.

The NVIDIA C compiler \( \text{nvcc} \) separates phases at compilation:
- Code for the host is compiled on host’s standard C compilers and runs as ordinary CPU process.
- The device code is written in C with keywords for data parallel functions and further compiled by \( \text{nvcc} \).
execution of a CUDA program

CPU code

kernel<<<numb_blocks,numb_threads_per_block>>>(args)

CPU code

grid

block 0  block 1  block \( N - 1 \)
stages in a CUDA program

For the matrix multiplication $C = A \cdot B$:

1. Allocate device memory for $A$, $B$, and $C$.
2. Copy $A$ and $B$ from the host to the device.
3. Invoke the kernel to have device do $C = A \cdot B$.
4. Copy $C$ from the device to the host.
5. Free memory space on the device.
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Consider a 3-by-5 matrix stored row-wise (as in C):

\[
\begin{array}{cccccc}
  a_{0,0} & a_{0,1} & a_{0,2} & a_{0,3} & a_{0,4} \\
  a_{1,0} & a_{1,1} & a_{1,2} & a_{1,3} & a_{1,4} \\
  a_{2,0} & a_{2,1} & a_{2,2} & a_{2,3} & a_{2,4} \\
\end{array}
\]

We will store a matrix as a one dimensional array.
generating a random matrix

```c
#include <stdlib.h>

__host__ void randomMatrix ( int n, int m, float *x, int mode )
/*
 * Fills up the n-by-m matrix x with random
 * values of zeroes and ones if mode == 1,
 * or random floats if mode == 0. */
{
    int i, j, r;
    float *p = x;

    for(i=0; i<n; i++)
        for(j=0; j<m; j++)
        {
            if(mode == 1)
                r = rand() % 2;
            else
                r = ((float) rand())/RAND_MAX;
            *(p++) = (float) r;
        }
}
```
writing a matrix

#include <stdio.h>

__host__ void writeMatrix ( int n, int m, float *x )
/*
  * Writes the n-by-m matrix x to screen. */
{
  int i, j;
  float *p = x;

  for(i=0; i<n; i++, printf("\n"))
    for(j=0; j<m; j++)
      printf(" %d", (int) *(p++));
}
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4. Examining Performance
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assigning inner products to threads

Consider a 3-by-4 matrix $A$ and a 4-by-5 matrix $B$:

\[
\begin{array}{cccc}
  a_{0,0} & a_{0,1} & a_{0,2} & a_{0,3} \\
  a_{1,0} & a_{1,1} & a_{1,2} & a_{1,3} \\
  a_{2,0} & a_{2,1} & a_{2,2} & a_{2,3}
\end{array} \quad \begin{array}{cccc}
  b_{0,0} & b_{0,1} & b_{0,2} & b_{0,3} & b_{0,4} \\
  b_{1,0} & b_{1,1} & b_{1,2} & b_{1,3} & b_{1,4} \\
  b_{2,0} & b_{2,1} & b_{2,2} & b_{2,3} & b_{2,4} \\
  b_{3,0} & b_{3,1} & b_{3,2} & b_{3,3} & b_{3,4}
\end{array}
\]

\[
\begin{array}{cccccccccc}
  c_{0,0} & c_{0,1} & c_{0,2} & c_{0,3} & c_{0,4} & c_{1,0} & c_{1,1} & c_{1,2} & c_{1,3} & c_{1,4} \\
  c_{2,0} & c_{2,1} & c_{2,2} & c_{2,3} & c_{2,4}
\end{array}
\]

The $i = blockIdx.x \times blockDim.x + threadIdx.x$ determines what entry in $C = A \cdot B$ will be computed:

- the row index in $C$ is $i$ divided by 5 and
- the column index in $C$ is the remainder of $i$ divided by 5.
the kernel function

`__global__ void matrixMultiply`

```c
(int n, int m, int p, float *A, float *B, float *C)
{
    int i = blockIdx.x*blockDim.x + threadIdx.x;
    C[i] = 0.0;
    int rowC = i/p;
    int colC = i%p;
    float *pA = &A[rowC*m];
    float *pB = &B[colC];
    for(int k=0; k<m; k++)
    {
        pB = &B[colC+k*p];
        C[i] += (*pA++)*(*pB);
    }
}
```
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running the program

```bash
$ /tmp/matmatmul 3 4 5 1
a random 3-by-4 0/1 matrix A :
  1 0 1 1
  1 1 1 1
  1 0 1 0
a random 4-by-5 0/1 matrix B :
  0 1 0 0 1
  0 1 1 0 0
  1 1 0 0 0
  1 1 0 1 0
the resulting 3-by-5 matrix C :
  2 3 0 1 1
  2 4 1 1 1
  1 2 0 0 1
$```

Introduction to Supercomputing (MCS 572)
Data Parallelism & Matrix Multiplication

L-31 2 November 2016 18 / 32
the main program — command line arguments

```c
int main ( int argc, char*argv[] )
{
    if(argc < 4)
    {
        printf("call with 3 arguments :\n");
        printf("dimensions n, m, and p\n");
    }
    else
    {
        int n = atoi(argv[1]); /* number of rows of A */
        int m = atoi(argv[2]); /* number of columns of A */
        int p = atoi(argv[3]); /* and number of rows of B */
        int mode = atoi(argv[4]); /* number of columns of B */
        int mode = atoi(argv[4]); /* 0 no output, 1 show output */
        if(mode == 0)
            srand(20140331)
        else
            srand(time(0));
    }
}
```

Introduction to Supercomputing (MCS 572)  Data Parallelism & Matrix Multiplication
allocating memories

```c
float *Ahost = (float*)calloc(n*m,sizeof(float));
float *Bhost = (float*)calloc(m*p,sizeof(float));
float *Chost = (float*)calloc(n*p,sizeof(float));
randomMatrix(n,m,Ahost,mode);
r
```
/* copy matrices A and B from host to the device */
cudaMemcpy(Adevice, Ahost, sA, cudaMemcpyHostToDevice);
cudaMemcpy(Bdevice, Bhost, sB, cudaMemcpyHostToDevice);

/* kernel invocation launching n*p threads */
matrixMultiply<<<n*p,1>>>(n, m, p,
    Adevice, Bdevice, Cdevice);

/* copy matrix C from device to the host */
cudaMemcpy(Chost, Cdevice, sC, cudaMemcpyDeviceToHost);
/* freeing memory on the device */
cudaFree(Adevice); cudaFree(Bdevice); cudaFree(Cdevice);
if (mode == 1)
{
    printf("the resulting %d-by-%d matrix C : \n", n, p);
    writeMatrix(n, p, Chost);
}
return 0;
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using threadIdx.x and threadIdx.y

Instead of a one dimensional organization of the threads in a block we can make the \((i,j)\)-th thread compute \(c_{i,j}\).

The main program is then changed into

```c
/* kernel invocation launching n*p threads */
dim3 dimGrid(1,1);
dim3 dimBlock(n,p);
matrixMultiply<<<dimGrid,dimBlock>>>(
    (n,m,p,Adevice,Bdevice,Cdevice);
```

The above construction creates a grid of one block. The block has \(n \times p\) threads:

- \(\text{threadIdx.x}\) will range between 0 and \(n - 1\), and
- \(\text{threadIdx.y}\) will range between 0 and \(p - 1\).
the new kernel

__global__ void matrixMultiply
( int n, int m, int p, float *A, float *B, float *C )
/*
* Multiplies the n-by-m matrix A
* with the m-by-p matrix B into the matrix C.
* The (i,j)-th thread computes the (i,j)-th element of C.
*
{
  int i = threadIdx.x;
  int j = threadIdx.y;
  int ell = i*p + j;
  C[ell] = 0.0;
  float *pB;
  for(int k=0; k<m; k++)
  {
    pB = &B[j+k*p];
    C[ell] += A[i*m+k] * (*pB);
  }
}
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Performance analysis

Performance is often expressed in terms of flops.

- 1 flops = one floating-point operation per second;
- use `perf`: Performance analysis tools for Linux
- run the executable, with `perf stat -e`
  with the events following the `-e` flag
  we count the floating-point operations.

For the Intel Sandy Bridge in `kepler` the codes are

- 530110 : FP_COMP_OPS_EXE:X87
- 531010 : FP_COMP_OPS_EXE:SSE_FP_PACKED_DOUBLE
- 532010 : FP_COMP_OPS_EXE:SSE_FP_SCALAR_SINGLE
- 534010 : FP_COMP_OPS_EXE:SSE_PACKED_SINGLE
- 538010 : FP_COMP_OPS_EXE:SSE_SCALAR_DOUBLE

Executables are compiled with the option `-O2`. 
performance of one CPU core

$ perf stat -e r530110 -e r531010 -e r532010 -e r534010 -e r538010 ./matmatmul0 745 745 745 0$

Performance counter stats for './matmatmul0 745 745 745 0':

1,668,710 r530110
0 r531010
2,478,340,803 r532010
0 r534010
0 r538010

1.033291591 seconds time elapsed

$ Did 2,480,009,513 operations in 1.033 seconds:

⇒ (2,480,009,513/1.033)/(2^{30}) = 2.23GFlops.
performance on the K20C

```
$ perf stat -e r530110 -e r531010 -e r532010 -e r534010 \n   -e r538010 ./matmatmul1 745 745 745 0

Performance counter stats for './matmatmul1 745 745 745 0':

    160,925 r530110
        0 r531010
    2,306,222 r532010
        0 r534010
        0 r538010

    0.663709965 seconds time elapsed
```

```
$ time ./matmatmul1 745 745 745 0

real        0m0.631s
user        0m0.023s
sys         0m0.462s
```

The dimension 745 is too small for the GPU to be able to improve much.
increasing the dimension

$ perf stat -e r530110 -e r531010 -e r532010 -e r534010 \ 
  -e r538010 ./matmatmul0 4000 4000 4000 0

Performance counter stats for './matmatmul0 4000 4000 4000 0':

        48,035,278 r530110
            0 r531010
   267,810,771,301 r532010
            0 r534010
            0 r538010

171.33443720 seconds time elapsed

$ See if we can speedup the computations with the GPU...
running on the K20C

$ perf stat -e r530110 -e r531010 -e r532010 -e r534010
   -e r538010 ./matmatmul 4000 4000 4000 0

Performance counter stats for './matmatmul 4000 4000 4000 0':

<table>
<thead>
<tr>
<th>Counter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>r530110</td>
<td>207,682</td>
</tr>
<tr>
<td>r531010</td>
<td>0</td>
</tr>
<tr>
<td>r532010</td>
<td>64,222,441</td>
</tr>
<tr>
<td>r534010</td>
<td>0</td>
</tr>
<tr>
<td>r538010</td>
<td>0</td>
</tr>
</tbody>
</table>

1.011284551 seconds time elapsed

$

Speedup: 171.334/1.011 = 169.

Counting flops, $f = 267,810,771,301$

- $t_{cpu} = 171.334: f/t_{cpu}/(2^{30}) = 1.5$ GFlops.
- $t_{gpu} = 1.011: f/t_{gpu}/(2^{30}) = 246.7$ GFlops.
running on pascal, on the P100

On a larger GPU, we need to scale the problem:

\[
\begin{array}{|c|c|c|}
\hline
n = 2^k & n & \text{time} \\
\hline
2^{12} & 4096 & 1.33s \\
2^{13} & 8192 & 2.32s \\
2^{14} & 16384 & 6.24s \\
2^{15} & 32768 & 22.76s \\
\hline
\end{array}
\]

Matrix-Matrix multiplication is an \( O(n^3) \) operation: doubling the dimension, we expect the time increase eightfold.

A very rough estimate on the flops count (single precision floats):
- For \( n = 4,000 \), the flop count is \( f = 267,810,771,301 \).
- To scale to \( n = 2^{15} \): \( n \times 8 \), so \( F = 512 \times f \).
- In 22.76 seconds, so flops is \( (F/22.76)/(2^{30}) = 5610.8 \).

So we estimate the performance at 5.6 TeraFlops for \( n = 32,000 \).
We covered more of chapter 3 in the book of Kirk & Hwu.

1. Modify `matmatmul0.c` and `matmatmul1.cu` to work with doubles instead of floats. Examine the performance.
2. Modify `matmatmul2.cu` to use double indexing of matrices, e.g.: \( C[i][j] += A[i][k] \times B[k][j] \).
3. Compare the performance of `matmatmul1.cu` and `matmatmul2.cu`, taking larger and larger values for \( n, m, \) and \( p \). Which version scales best?