Announcements

- MPI assignment due last night
  - Questions?
- Assignment 2 on Tools posted yesterday
  - Questions?
CUDA

- Software ecosystem for NVIDIA GPUs
- Language for programming GPUs
  - C++ language extension
  - *.cu files
- NVCC compiler

```bash
> nvcc -o saxpy --generate-code arch=compute_80,code=sm_80 saxpy.cu
> ./saxpy
```

Alan Sussman (from Daniel Nichols)
__global__ void saxpy(float *x, float *y, float alpha) {
    int i = threadIdx.x;
    y[i] = alpha * x[i] + y[i];
}

int main() {
    ...
    saxpy<<<1, N>>>(x, y, alpha);
    ...
}
Possible Issues?

```c
__global__ void saxpy(float *x, float *y, float alpha) {
    int i = threadIdx.x;
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}

int main() {
    ...
    saxpy<<<1, N>>>(x, y, alpha);
    ...
}
```

What happens when:
- N > 1024?
- N > # device threads?
Multiple Blocks

__global__ void saxpy(float *x, float *y, float alpha, int N) {
    int i = blockDim.x * blockIdx.x + threadIdx.x;
    if (i < N)
        y[i] = alpha * x[i] + y[i];
}

...  
int threadsPerBlock = 512;
int numBlocks = N / threadsPerBlock + (N % threadsPerBlock != 0);
saxpy<<<numBlocks, threadsPerBlock>>>(x, y, alpha, N);
__global__ void saxpy(float *x, float *y, float alpha, int N) {
    int i0 = blockDim.x * blockIdx.x + threadIdx.x;
    int stride = blockDim.x * gridDim.x;

    for (int i = i0; i < N; i += stride)
        y[i] = alpha*x[i] + y[i];
}
Grid and Block Dimensions

- # of blocks and threads per block can be 3-vectors
- Useful for algorithms with 2d & 3d data layouts
Grid and Block Dimensions

GRID

| gridDim.x | gridDim.y | gridDim.z |

BLOCK

| blockDim.x | blockDim.y | blockDim.z |

THREAD

Alan Sussman (from Daniel Nichols)
Grid and Block Dimensions

dim3 threadsPerBlock(16, 16);

dim3 numBlocks(M/threadsPerBlock.x + (M % threadsPerBlock.x != 0),
N/threadsPerBlock.y + (N % threadsPerBlock.y != 0));

matrixAdd<<<numBlocks, threadsPerBlock>>>(X, Y, alpha, M, N);
Grid and Block Dimensions

Each block is 16x16 threads.

dim3 threadsPerBlock(16, 16);
dim3 numBlocks(M/threadsPerBlock.x + (M % threadsPerBlock.x != 0),
                 N/threadsPerBlock.y + (N % threadsPerBlock.y != 0));

matrixAdd<<<numBlocks, threadsPerBlock>>>(X, Y, alpha, M, N);
Grid and Block Dimensions

The grid is \([M/16] \times [N/16]\) blocks.

\[
\text{dim3 threadsPerBlock}(16, 16);
\]
\[
\text{dim3 numBlocks} (\frac{M}{\text{threadsPerBlock}.x} + (M \mod \text{threadsPerBlock}.x != 0),
\frac{N}{\text{threadsPerBlock}.y} + (N \mod \text{threadsPerBlock}.y != 0));
\]
\[
\text{matrixAdd}<<<\text{numBlocks}, \text{threadsPerBlock}>>>(X, Y, \alpha, M, N);
\]
```c
__global__ void matrixAdd(float **X, float **Y, float alpha, int M, int N)
{
    int i = blockDim.x * blockIdx.x + threadIdx.x;
    int j = blockDim.y * blockIdx.y + threadIdx.y;

    if (i < M && j < N)
        Y[i][j] = alpha*X[i][j] + Y[i][j];
}
```
Questions?
Matrix Multiply

- Standard matrix multiply
- How can we parallelize?

```c
for (i=0; i<M; i++)
    for (j=0; j<N; j++)
        for (k=0; k<P; k++)
            C[i][j] += A[i][k]*B[k][j];
```
Matrix Multiply

- $C_{ij}$ can be computed independent of other values of $C$
- 2-D thread decomposition
- Thread $(i, j)$ computes $C_{ij}$

Matrix Multiply

- Launch \(M \times N\) threads
- Thread \((i,j)\) computes \(C_{ij}\)

\[
\text{dim3 threadsPerBlock (BLOCK\_SIZE, BLOCK\_SIZE);} \\
\text{dim3 numBlocks(M/threadsPerBlock.x + (M\%threadsPerBlock.x != 0),} \\
\text{N/threadsPerBlock.y + (N\%threadsPerBlock.y != 0));} \\
\text{matmul<<<numBlocks, threadsPerBlock>>>(C, A, B, M, P, N);} \\
\]
Matrix Multiply

__global__ void matmul(double *C, double *A, double *B, size_t M, size_t P, size_t N) {

    int i = blockDim.x*blockIdx.x + threadIdx.x;
    int j = blockDim.y*blockIdx.y + threadIdx.y;

    if (i < M && j < N) {
        for (int k = 0; k < P; k++) {
            C[i*N+j] += A[i*P+k]*B[k*N+j];
        }
    }
}

Compute $C_{ij}$
Issues?
Issues?

- Poor data re-use
  - Every value of A & B is loaded from global memory
Issues?

● Poor data re-use
  ○ Every value of A & B is loaded from global memory
  ○ A is read N times
  ○ B is read M times
Issues?

● Poor data re-use
  ○ Every value of A & B is loaded from global memory
    ○ A is read N times
    ○ B is read M times

● How can we improve data re-use?
Announcements

- Assignment 2 on Tools due Thursday, 11:59PM
  - Questions?
- No class Thursday, so work on the assignment!
  - No office hour on Wednesday for me, office hour on Thursday is on Zoom instead of in-person
Shared Memory

- **Local**
  - thread only
- **Shared**
  - threads in block
- **Global**
  - all threads

Alan Sussman (from Daniel Nichols)
Shared Memory

- `__shared__`
  - Denotes shared memory
- `__syncthreads()`
  - Synchronizes all threads in block
__global__ void reverse(int *vec) {
    __shared__ int sharedVec[N];

    int idx = threadIdx.x;
    int idxReversed = N - idx - 1;

    sharedVec[idx] = vec[idx];
    __syncthreads();
    vec[idx] = sharedVec[idxReversed];
}
Reversing with Shared Memory

```c
__global__ void reverse(int *vec) {
  __shared__ int sharedVec[N];

  int idx = threadIdx.x;
  int idxReversed = N - idx - 1;

  sharedVec[idx] = vec[idx];
  __syncthreads();
  vec[idx] = sharedVec[idxReversed];
}
```

Allocate N ints in block.
__global__ void reverse(int *vec) {
    __shared__ int sharedVec[N];

    int idx = threadIdx.x;
    int idxReversed = N - idx - 1;

    sharedVec[idx] = vec[idx];
    __syncthreads();
    vec[idx] = sharedVec[idxReversed];
}
Matrix Multiply with Shared Memory

- How can we speed up matrix multiply with shared memory?
Matrix Multiply with Shared Memory

- **Data Reuse**
  - A is read \( N \) times
  - B is read \( M \) times
Matrix Multiply with Shared Memory

- Block computation
- Each block computes submatrix of $C$
- Save reused values in shared memory


Alan Sussman (from Daniel Nichols)
Matrix Multiply with Shared Memory

- Compute $C = AB + C$
Matrix Multiply with Shared Memory

- Block \((i, j)\) computes \(C_{ij}\) submatrix
  - Save A & B submatrices into shared memory
Matrix Multiply with Shared Memory

- Block \((i, j)\) computes \(C_{ij}\) submatrix
  - Save \(A\) & \(B\) submatrices into shared memory
  - Accumulate partial dot product into \(C\)
Matrix Multiply with Shared Memory

- Block \((i, j)\) computes \(C_{ij}\) submatrix
  - Save \(A\) & \(B\) submatrices into shared memory
  - Accumulate partial dot product into \(C\)
Matrix Multiply with Shared Memory

- Block (i, j) computes $C_{ij}$ submatrix
  - Save A & B submatrices into shared memory
  - Accumulate partial dot product into C
Matrix Multiply with Shared Memory

- A is read N / block_size times
- B is read M / block_size times
- Data reads from global memory are reduced by O(block size)

Reference Implementation:
https://github.com/NVIDIA/cuda-samples/blob/master/Samples/matrixMul/matrixMul.cu

Alan Sussman (from Daniel Nichols)
How much faster is it?

Compare GPU Algorithms

<table>
<thead>
<tr>
<th>Algorithm</th>
<th>Time* (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Simple CPU</td>
<td>170.898</td>
</tr>
<tr>
<td>Simple GPU</td>
<td>1.997</td>
</tr>
<tr>
<td>Shared Memory</td>
<td>0.091</td>
</tr>
<tr>
<td>CuBLAS</td>
<td>0.017</td>
</tr>
</tbody>
</table>

A, B are 2048x2048
* on DeepThought2
Questions?

Alan Sussman (from Daniel Nichols)
Profiling GPUs

- HPCToolkit + Hatchet
  - In addition to normal HPCToolkit commands
    - `hpcrun -e gpu=nvidia ...
    - `hpcstruct <measurements_dir`
- NSight
  - NVIDIA profiling suite
NSight

- nsys command to profile
  - nsys profile -t cuda <executable> <args>
  - Outputs .qdrep file
- View profile in NSight GUI
  - nsys-ui report1.qdrep

NSight


Alan Sussman (from Daniel Nichols)
Streams

- Kernels execute in streams
- Stream is passed to kernel invocation
- Streams can execute concurrently

```c
cudaStream_t stream;
...
kernel<<<grid, block, 0, stream>>>(x, b);
```

More info
Streams

Serial Model

H2D Engine 0
Kernel Engine 0
D2H Engine 0

Concurrent Model

H2D Engine 1 2 3 4
Kernel Engine 1 2 3 4
D2H Engine 1 2 3 4

Image from https://leimao.github.io/blog/CUDA-Stream/
Unified Memory

- Data is on both GPU and CPU
- GPU takes care of synchronization
- Incurs small overhead

```c
void sortfile(FILE *fp, int N) {
    char *data;
    cudaMallocManaged(&data, N);
    fread(data, 1, N, fp);
    qsort<<<...>>>(data, N, 1, compare);
    cudaDeviceSynchronize();
    ... use data on CPU ...
    cudaFree(data);
}
```


Alan Sussman (from Daniel Nichols)
GPU Programming w/Libraries
GPU Programming w/Libraries

- Linear Algebra
  - CuBLAS, MAGMA, CUTLASS, Eigen, CuSPARSE, ...

Alan Sussman (from Daniel Nichols)
GPU Programming w/Libraries

- **Linear Algebra**
  - CuBLAS, MAGMA, CUTLASS, Eigen, CuSPARSE, …
- **Signal Processing**
  - CuFFT, ArrayFire, …
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  - OpenCV, FFmpeg, OpenGL, …
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  - CuFFT, ArrayFire, …
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  - CuDNN, TensorRT, …
- Graphics
  - OpenCV, FFmpeg, OpenGL, …
- Algorithms and Data Structures
  - Thrust, Raja, Kokkos, OpenACC, OpenMP, …
An Example: Raja

RAJA::View<double, RAJA::Layout<DIM>> Aview(A, N, N);
RAJA::View<double, RAJA::Layout<DIM>> Bview(B, N, N);
RAJA::View<double, RAJA::Layout<DIM>> Cview(C, N, N);

RAJA::forall<RAJA::loop_exec>( row_range, [=](int row) {
    RAJA::forall<RAJA::loop_exec>( col_range, [=](int col) {
        double dot = 0.0;
        for (int k = 0; k < N; ++k) {
            dot += Aview(row, k) * Bview(k, col);
        }
        Cview(row, col) = dot;
    });
});

See https://raja.readthedocs.io/en/v0.13.0/tutorial/matrix_multiply.html
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Kernel Execution Policy
- OpenMP
- CUDA
- AMD GPU
- Serial
Big Picture

- When to use GPUs?
Big Picture

- When to use GPUs?
  - Data parallel tasks & lots of data
  - Performance/$$$ and time-to-solution

Alan Sussman (from Daniel Nichols)
Big Picture

● When to use GPUs?
  ○ Data parallel tasks & lots of data
  ○ Performance/$$$ and time-to-solution

● What software/algorithm to use?
Big Picture

- When to use GPUs?
  - Data parallel tasks & lots of data
  - Performance/$$$ and time-to-solution

- What software/algorith to use?
  - Performance critical
    - Native languages
  - Development time & maintainability
    - higher level APIs