GPU programming in CUDA: Advanced topics in CUDA

Lukas Einkemmer
Department of Mathematics
University of Innsbruck

PRACE Autumn School, Innsbruck
Link to slides: `http://www.einkemmer.net/training.html`

Shared memory

Reminder on Caches

Cache is a type of **fast, but small, memory** that accelerates repeated access to the same memory location.

- Usually, i.e. on CPUs, completely transparent to the programmer.

On the GPU we can explicitly control the L1 cache.

- **Shared memory**.

Often essential to obtain good performance for memory bound problems.

Shared memory

The `__shared__` keyword declares a variable/array that resides in shared memory.

Such variables are **shared among the threads in a block**.

- No communication between blocks is possible using shared memory.

Example using shared memory

```
__global__ void k_stencil(double* x, double* y, int n) {
    int i = threadIdx.x + blockDim.x*blockIdx.x;

    // Local_x is an array in shared memory.
    __shared__ double local_x[1024];

    // Each thread loads its value of x into local_x that is shared
    if(i < n) local_x[threadIdx.x] = x[i];

    __syncthreads();

    if(threadIdx.x > 0 && threadIdx.x < blockDim.x-1)
        y[i] = local_x[threadIdx.x+1]-local_x[threadIdx.x-1];
    else if(threadIdx.x == 0 && i > 0)
        y[i] = local_x[threadIdx.x+1]-x[i-1];
    else if(threadIdx.x == blockDim.x-1 && i < n-1)
        y[i] = x[i+1] - local_x[threadIdx.x-1];
}
```

Synchronization

The `__syncthreads()` function acts as a barrier for all threads in a block.

- Threads in different blocks are not affected.

General philosophy: Threads in the same block can synchronize and exchange data (via shared memory).

- No synchronization between blocks in a single kernel.

Recommendation: If you need to synchronize between blocks rethink your work and data distribution.

- You might have a problem that does not map very well to the GPU hardware.

Dynamic shared memory

What about dynamic shared memory?

```
__global__ void k_sum(double* x, double* out, int n) {
    extern __shared__ char shared_mem[];
}

k_sum<<<num_blocks, num_threads, shared_mem_size>>>
    (d_x, d_out, n);
```

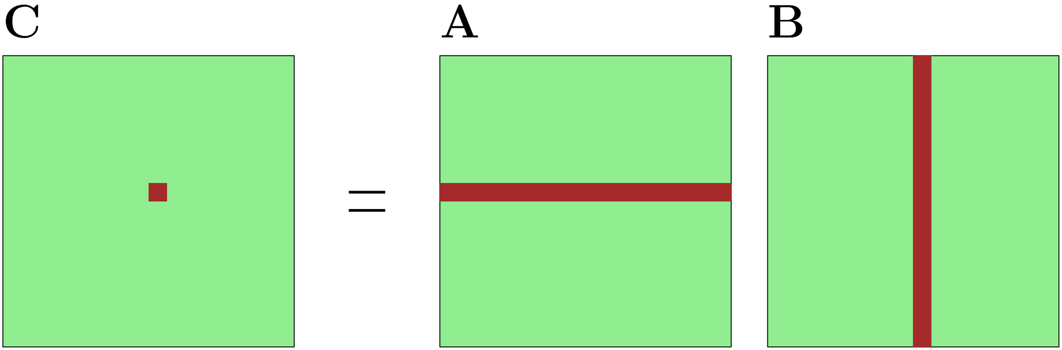
The argument `shared_mem_size` specifies the size (in bytes) of the array `shared_mem`.

Only one such dynamic shared memory block is allowed per kernel.

Matrix-matrix multiplication

Matrix-matrix multiplication

$$C_{i,j} = \sum_k A_{i,k} B_{k,j}.$$



Straightforward implementation

Each thread computes one element of the output matrix $C_{i,j}$.

```
__global__
void matmul(long n, double* A, double* B, double* C) {
    long i = blockIdx.x*blockDim.x + threadIdx.x;
    long j = blockIdx.y*blockDim.y + threadIdx.y;

    double val=0.0;
    for(long k=0;k<n;k++)
        val += A[i+k*n]*B[k+j*n];

    C[i+j*n] = val;
}
```

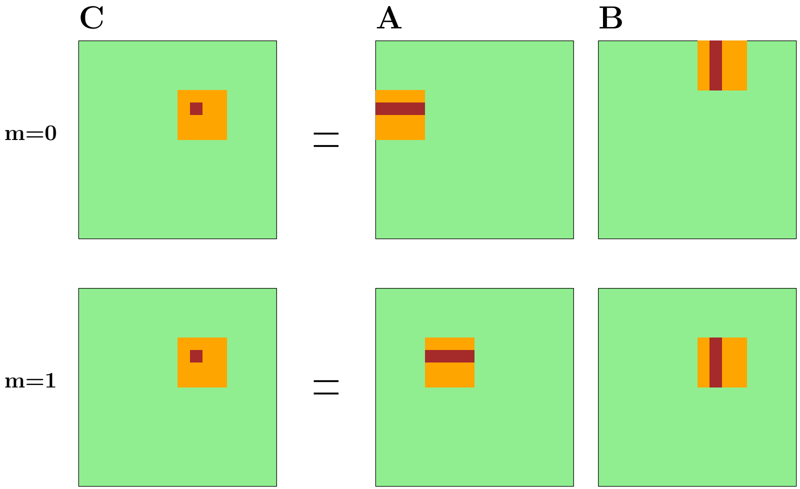
On the V100 (n=8192) we obtain 2.2 TFLOPS.

- Theoretical peak of 15 TFLOPS.
- Arithmetic operations $\mathcal{O}(n^3)$ vs memory accesses $\mathcal{O}(n^2)$.

Better algorithm

Each block computes a submatrix.

- Data loaded once and then stored in shared memory.



Implementation

```
__global__
void matmul_fast(long n, float* A, float* B, float* C) {
    long i = threadIdx.x; long bi = blockIdx.x;
    long j = threadIdx.y; long bj = blockIdx.y;

    // loop over all sub-matrices
    float val = 0.0;
    for(long m=0;m<n/BS;m++) {
        __shared__ float block_A[BS*BS];
        __shared__ float block_B[BS*BS];

        // load block into shared memory
        block_A[i+BS*j] = A[bi*BS+i + n*(m*BS+j)];
        block_B[i+BS*j] = B[m*BS+i  + n*(bj*BS+j)];

        // wait until all threads have caught up
        __syncthreads();
```

Implementation

```
        // compute the (sub-)matrix-matrix product
        for(long k=0;k<BS;k++)
            val += block_A[i+BS*k]*block_B[k+BS*j];

        // make sure that all threads are finished before
        // next loop iteration starts.
        __syncthreads();
    }

    // update result in global memory
    C[bi*BS+i + n*(bj*BS+j)] = val;
}
```

On the V100 (n=8192) we obtain 4.2 TFLOPS.

- Improvement by approximately a factor of two.

Exercise

Given a vector v in GPU memory compute $\sum_i v_i$.

- Start from `exercise-advanced-einkemmer.cu`.

Use shared memory to perform the sum in each block.

- Each block writes its (local) result to global memory.
- Repeat this procedure until you obtain the entire sum.

Once your code produces the correct result, time your code and report its performance.