



Exa-SofT

Introduction aux GPUs, à la programmation CUDA

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- Programmation particulière
 - Parallélisme massif !
 - Mémoire séparée (la plupart du temps)
- Développement particulier
 - Compilation différente
 - Lancement par offload logiciel
 - On ne peut pas juste recompiler
 - Outils de débuggage différents



















	L1 Instruction Cache																
			L0 Instruction Cache														
Warp Scheduler (32 thread/clk)									Warp Scheduler (32 thread/clk)								
Dispatch Unit (32 thread/clk)									Dispatch Unit (32 thread/clk)								
Register File (16,384 x 32-bit)									Register File (16,384 x 32-bit)								
FP64	INT	INT	FP32	FP32					FP	64	INT	INT	FP32	FP32			
FP64	INT	INT	FP32	FP32					FP	64	INT	INT	FP32	FP32			
FP64	INT	INT	FP32	FP32				F	FP	64	INT	INT	FP32	FP32			
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FP64	INT	INT	FP32	FP32					FP64		INT	INT	FP32	FP32			
FP64	INT	INT	FP32	FP32					FP	64	INT	INT	FP32	FP32			
FP64	INT	INT	FP32	FP32				FP64		64	INT	INT	FP32	FP32			
LD/ LD/ ST ST	LD/ ST	LD/ ST	LD/ ST	LD/ ST	LD/ ST	LD/ ST	SFU		LD/ ST	LD/ ST	LD/ ST	LD/ ST	LD/ ST	LD/ ST	LD/ ST	LD/ ST	SFU



Massive parallelism ! Example: V100

- 5,120 CUDA cores, structured in SM, TPC, GPC, ...
 - Parallelism to be structured
 - And massive to overlap memory access
- SP: ~16TFlop/s
- DP: ~8TFlop/s
- HBM Memory: ~900GB/s
- (and not counting the tensor cores)

Basic block: Streaming Multiprocessor (SM)

- = Cluster of streaming processors (~core)
- Local memory sharing
- Synchronization
- 64KB of registers
- hardware threads
 - Creation/destruction is free !



Only one instruction dispatch unit per SM

- All cores execute the same instruction at the same clock cycle
- On different data \Rightarrow SIMD
- Takes several cycles to fetch&decode



Only one instruction dispatch unit per SM

- All cores execute the same instruction at the same clock cycle
- On different data \Rightarrow SIMD
- Takes several cycles to fetch&decode
- ⇒ overlap by running yet more threads running the same instruction
 - Warp = 32 threads



Only one instruction dispatch unit per SM

- Loading data from global memory takes cycles
- ⇒ overlap by running yet more threads
 - 128 are enough to hide memory latency



Threads, threads, threads...

- But they are trivial to create
- Example: vector scaling



But hierarchy of SM

• Thread scheduling needs structure : blocks

```
static __global__ void vector_mult_cuda(unsigned n, float *val, float factor)
ł
        unsigned i = blockIdx.x*blockDim.x + threadIdx.x;
                                                                    Two-dimension
        if (i < n) val[i] *= factor;</pre>
                                                                      indexing
}
                                                                    (can be three)
extern "C" voi Compensate round-up signed n, float *val, float factor)
ł
        unsigned threads per block = 64;
        unsigned nblocks = (n + threads_per_block-1) / threads_per_block;
        vector_mult_cuda<<<nblocks,threads_per_block,0>>>(n, val, *factor);
}
```

Threads, threads, threads...

- Trivial to create
 - Massive parallelism
 - Forget about for loops
- Thread scheduling needs structure : blocks
 - How large? Depends on
 - the GPU generation,
 - available parallelism, ...

Thread divergence

static global void vector mult cuda(unsigned n, float *val, float factor) { unsigned i = blockIdx.x*blockDim.x + threadIdx.x; if (i < n && i % 2 == 0) val[i] *= factor;</pre> } Only half the threads actually work \Rightarrow 2x parallelism loss Related to warps; depends on GPU generation

Memory coalescing

```
static __global__ void vector_mult_cuda(unsigned n, float *val, float factor)
{
    unsigned i = blockIdx.x*blockDim.x + threadIdx.x;
    val[i*2 ] *= factor;
    val[i*2+1] *= factor;
}
```

Performance is weak : accesses are non-coalesced

Memory coalescing

```
static __global__ void vector_mult_cuda(unsigned n, float *val, float factor)
{
    unsigned i = blockIdx.x*blockDim.x + threadIdx.x;
    val[i*2 ] *= factor;
    val[i*2+1] *= factor;
}
```

Performance is weak : accesses are non-coalesced

Memory coalescing

```
static __global__ void vector_mult_cuda(unsigned n, float *val, float factor)
{
    unsigned i = blockIdx.x*blockDim.x + threadIdx.x;
    unsigned nthreads = blockDim.x * blockDim.y;
    val[ i] *= factor;
    val[nthreads + i] *= factor;
}
```

Accesses are coalesced

Memory coalescing

```
static __global__ void vector_mult_cuda(unsigned n, float *val, float factor)
{
    unsigned i = blockIdx.x*blockDim.x + threadIdx.x;
    unsigned nthreads = blockDim.x * blockDim.y;
    val[ i] *= factor;
    val[nthreads + i] *= factor;
}
```

Accesses are coalesced

Memory coalescing

- Depends on the GPU generation
- Better use structures of arrays
 - E.g. all threads get the temperature, then the pression, etc.
- For the global memory
- Not for the local shared memory
 - Has to be allocated explicitly

Summary : requires

- Massive parallelism
- Taking care of divergence
- Taking care of memory coalescing
 - Or taking care of using the local shared memory
- And other details I don't have time to explain :)

If you can avoid writing kernels it's best...



But we need to get data onto the GPU...

NumPEx Exascale computing Data management

- Allocate memory on the GPU
- Copy between GPU and CPU
 - For copy to be efficient, use cudaMallocHost for CPU memory
 - Pinned memory for DMA

```
void scal_func(unsigned n, float *val_cpu, float factor)
{
    float *val_gpu;
    cudaMalloc(&val_gpu, n * sizeof(float));
    cudaMemcpy(val_gpu, val_cpu, n * sizeof(float), cudaMemcpyHostToDevice);
    scal_cuda_func(n, val_gpu, factor);
    cudaMemcpy(val_cpu, val_gpu, n * sizeof(float), cudaMemcpyDeviceToHost);
}
```

Numpex Exascale computing Data management

But transfer takes time

- Overlap cudaMemcpy with another kernel execution
- Async variants of cuda operations, and poll or wait
- Use Streams for coordination

```
void scal_func(unsigned n, float *val_cpu, float factor)
{
    float *val_gpu;
    cudaMalloc(&val_gpu, n * sizeof(float));
    cudaMemcpy(val_gpu, val_cpu, n * sizeof(float), cudaMemcpyHostToDevice);
    scal_cuda_func(n, val_gpu, factor);
    cudaMemcpy(val_cpu, val_gpu, n * sizeof(float), cudaMemcpyDeviceToHost);
}
```

Numpex Exascale computing Data management

Or use cudaGraphs

- Express dependencies explicitly between cudaMemcpyAsync and kernel calls
- Let the GPU process the task graph

NumPEx Exascale computing Data management

Topology matters

- NVlink provides fast GPU-GPU transfers
- GPU-Direct provides fast NIC-GPU transfers
 - With CUDA-aware MPI implementation
- Beware of PCI topology
- Beware of NUMA topology



NumPEx Exascale computing Data management

Or use unified memory

- Pass managed pointers to kernels
- CUDA runtime handles transfers on the fly
- But CUDA runtime is mostly blind
 - On-demand migration, introduces latency
 - With cudaMemAdvise / cudaMemPrefetch hints, can be efficient



Numpex Exascale computing Data management

Summary

- HBM memory embedded in GPU
- Requires transfers
- To be pipelined with computation kernels
- If you can avoid managing this it's best...

NumPEx Exascale computing Conclusion

GPUs are beasts

- Require massive parallelism
 - With massive data accesses
- Optimizing is very involved
- Better delegate it to another software layer