Massive parallel programming on Graphics Processing Units and Applications (part 2)

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Plan

Install, notebook and documentation

- Install/use on Linux and Windows local machine
- Jupyter notebook and Google Colab
- Extensive documentation

GPU architecture and device query

- Runtime API and error handling
- GPU architecture
- GPU specifications

Hello World! and built-in variables

- Kernel and device functions
- “Hello World!” and fourth parallel granularity
- Different levels of synchronization

Addition of two arrays

- Main steps
- Indices, global memory and registers
- CPU timer vs. GPU timer

Real applications

- Monte Carlo simulation
- Partial Differential Equation simulation

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on Linux machines

Before Installation

- Check that you have a (Nvidia) GPU on which you can use CUDA: `lspci | grep -i nvidia`
- Verify Linux version: `uname -m && cat /etc/*release`

Installation steps

- gcc/g++ should be already available on your machine, otherwise install it
- Install CUDA: `https://developer.nvidia.com/cuda-downloads`
- Disabling Secure Boot on UEFI (BIOS)
- Add `/usr/local/cuda/bin` to `PATH` and `/usr/local/cuda/lib64` to `LD_LIBRARY_PATH`
- Any problem during installation or compilation? Check `https://docs.nvidia.com/cuda/cuda-installation-guide-linux/index.html` especially to deal with the conflicting installation

Compilation + Execution

- Compile `name.cu` using `nvcc name.cu -o nameex`
- The options `-arch=compute_Xx -code=sm_Yy` should be used sometimes
- For the compilation of various files, an example of a Makefile is also given
- Execute `nameex` using: `./nameex`

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on Windows machines

Before Installation

- Check that you have a (Nvidia) GPU on which you can use CUDA: `control /name Microsoft.DeviceManager`
- Verify Windows version: `winver`

Installation steps

- Install Visual Studio 2022 Community with C/C++ tools: `https://visualstudio.microsoft.com/downloads/`
- Install CUDA: `https://developer.nvidia.com/cuda-downloads`
- Disabling Secure Boot on UEFI (BIOS)
- Add the address of `cl` compiler to `Path`
- Perform register changes explained at 7:40 in the video `https://www.youtube.com/watch?v=8NtHDkUoN98`
- Additional information on `https://docs.nvidia.com/cuda/cuda-installation-guide-microsoft-windows/index.html`

Compilation + Execution

- Compile `name.cu` using `nvcc name.cu -o nameex`
- The options `-arch=compute_Xx -code=sm_Yy` should be used sometimes
- For the compilation of various files, an example using CMake is also given
- Execute `nameex` using: `nameex`

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Exercise session: local Jupyter or Google Colaboratory

Jupyter on a GPU CUDA-capable

- Perform the CUDA installation steps on either Linux or Windows machine
- Install Miniconda `https://docs.conda.io/projects/miniconda/en/latest/`
- Launch miniconda as administrator and create a virtual environment
- Activate the virtual environment then install everything you need, like: `conda install notebook` to install Jupyter notebook

Google Colab

- Have a Gmail account allows you to use Google Colab
- Open a new notebook
- Click on Runtime then change runtime type, choose T4 GPU
- To upload your Jupyter notebook, click on File.
- On the left toolbar, click on Files to upload your source code
- On your local machine, keep regular copies of the code written in Colab

Compilation + Execution

- Compile `name.cu` using `!nvcc name.cu -o nameex`
- Execute `nameex` using: `!./nameex`

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Most Important documents!

Very often use the documentation provided by NVIDIA, in particular:

- **CUDA_C_Programming_Guide**: Document necessary for mastering CUDA API and overall understanding of the GPU hardware architecture
- **CUDA_Runtime_API**: Document describing functions from CUDA API

Specific documents

- **CUDA C++ Best Practices guide**: The third most important
- **CUDA_Math_API**: mathematical functions and number formats
- Other Math libraries: cuBLAS, cuFFT, cuRAND, cuSPARSE, and others
- Optimizations on each architecture, debug and profile a code, and others

CUDA for Python

Just-in-Time compilation proposed by Numba JIT functions is the best option `https://numba.pydata.org/numba-doc/latest/cuda/kernels.html`

Libraries using CUDA

- The best option for Machine Learning: `https://pytorch.org/docs/stable/notes/cuda.html#cuda-semantics`
- For general purpose data science: `https://docs.rapids.ai/user-guide`

Forums and code samples

- For specific questions, you can use `https://forums.developer.nvidia.com/c/accelerated-computing/cuda/206`
- Some CUDA code samples are installed with the CUDA toolkit: `https://developer.nvidia.com/cuda-code-samples`
- Alternative forum `https://stackoverflow.com/questions/tagged/cuda`

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Runtime API

- Leads to simpler code when compared to Driver API, but it also lacks the level of control that the Driver API has
- The name of functions is prefixed by cuda like `cudaGetDeviceCount` and `cudaGetDeviceProperties`
- Functions return `cudaError_t` enum type with

`cudaSuccess = 0`	The API call returned with no errors
`cudaErrorInvalidValue = 1`	Some parameters passed to the call are not within an acceptable range of values
...	
`cudaErrorUnknown = 999`	Unknown internal error has occurred

- But some values are deprecated like `cudaErrorInvalidDevicePointer = 17`

Error handling

```c
#include <stdio.h>
// Function that catches the error
void testCUDA(cudaError_t error, const char *file, int line) {
    if (error != cudaSuccess) {
       printf("There is an error in file %s at line %d\n",
              file, line);
       exit(EXIT_FAILURE);
    }
}
// Has to be defined in the compilation in order to get
// the correct value of the macros __FILE__ and __LINE__
#define testCUDA(error) (testCUDA(error, __FILE__ , __LINE__))
```

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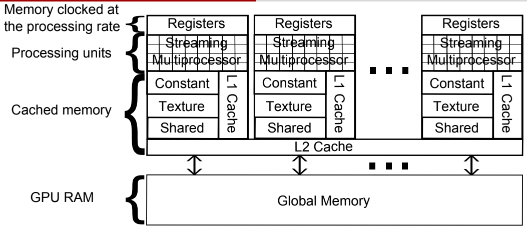


Multi-granularity parallelization

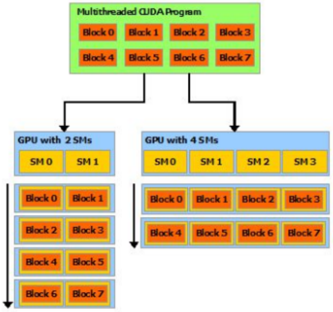
- Streaming processor: excutes threads
- Streaming multiprocessor: executes blocks
- Graphics Processing Cluster (new): executes grids

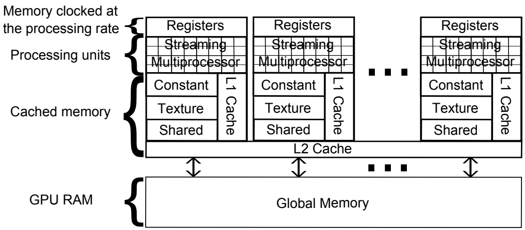
`empty_k<<<8,NTPB>>>();`

Depending on GPU capabilities

8 blocks of NTPB threads processed by either 2 SMs or 4 SMs

Figure from CUDA programming guide





GPU RAM

- contains global memory; values global to all threads
- could also contain local memory, values local to each thread

GPU cache

- Real cache: L1, L2 and shared memory
- Virtual cache: constant end texture memories

Main specifications Calling the function `cudaGetDeviceProperties (cudaDeviceProp *prop, int device)`

- `prop.totalGlobalMem, prop.sharedMemPerBlock, prop.regsPerBlock, prop.totalConstMem`
- `prop.major, prop.minor`
- `prop.maxThreadsPerBlock, prop.maxThreadsDim[3], prop.maxGridSize[3]`

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Function declaration and calling

Standard C functions

The same as for C or C++ programming

Kernel functions

- Called by the CPU and executed on the GPU
- Declared as `__global__ void myKernel (...) { ...; }`
- Called standardly by
  `myKernel<<<numBlocks, threadsPerBlock>>>(...);`
  where

  `numBlocks` should take into account the number of multiprocessors
  `threadsPerBlock` should take into account the warp size
- Dynamic parallelism: kernels can be called within kernels by the GPU and executed on the GPU

device functions

- Called by the GPU and executed on the GPU
- Declared as

```
__device__ void myDivFun (...)  { ...; }
__device__ float myDivFun (...)  { ...; }
```

- Called simply by `myDivFun(...)` but only within other device functions or kernels

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Hello World!

- `int printf(const char *format[, arg, ...])` can be called within a kernel function or a device function
- `printf` returns the number of arguments parsed instead of the number of characters printed
- `printf` executed by the GPU involves both the CPU and the GPU, thus the CPU should wait for GPU results before continuing
- `cudaDeviceSynchronize` makes the host wait for compute device to finish
- The number of printed `Hello World!` depends on the number of threads that execute `printf("Hello World!")`

Built-in variables

Known within functions excuted on GPU: threadIdx.x, blockDim.x, blockIdx.x, gridDim.x

- `threadIdx.x` identifies each thread within its block
- `blockIdx.x` identifies each block within its grid
- `blockDim.x` is the size of each block in terms of number of threads
- `gridDim.x` is the size of each grid in terms of number of blocks
- Also .y and .z are possible but not used in this course
- The order of printing `blockIdx.x` varies
- The order of printing `threadIdx.x` varies less as they grouped within warps of 32 threads:
  First warp, `threadIdx.x` ordered from 0 to 31
  Second warp, `threadIdx.x` ordered from 32 to 63
  and so on

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Synchronization of blocks

- Before compute capability 9.0, the NVIDIA Hopper GPU architecture, it is impossible to synchronize blocks without exiting the kernel function
- After compute capabilitty 9.0, it is possible to synchronize all the thread blocks in the same cluster, coscheduled on a single GPU Processing Cluster, using `cluster.sync()`

Synchronization of threads

Threads from the same block can be synchronized using `__syncthreads()`

Synchronization of warps

- Before compute capability 7.0, the NVIDIA Volta GPU architecture, warps used the same program counter shared amongst all 32 threads in the warp
- Before compute capability 7.0, no synchronization is needed between threads of the same warp
- For recent Nvidia architectures, of compute capability Y.y, one can force warp-synchronicity using the compilation option `-arch=compute_60 -code=sm_Yy` with Yy>60
- For recent Nvidia architectures, the synchronization of warps can be performed using `__syncwarp()`
- For any Nvidia architecture, long sequences of diverged execution by threads within the same warp should be avoided

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On CPU We want to add two large arrays of integers and put the result in a third one.

- Create a new file .cu, include `stdio.h` and `timer.h` in the top
- In the main function, allocate three arrays `a, b, c` using `malloc`
- Assign some values to `a` and `b`
- Using functions defined in `timer.h`, compute the execution time of adding `a` and `b`
- Free the CPU memory using `free`

On GPU We keep the same CPU code. For given values of *numBlocks* and *threadsPerBlock*, we want to perform an addition of *numBlocks* $\times$ *threadsPerBlock* integers

- Allocate `aGPU, bGPU, cGPU` on the GPU using `cudaMalloc`
- Transfer the values of `a, b` to `aGPU, bGPU` using `cudaMemcpy`
- Write the kernel that adds `aGPU` to `bGPU` and return the result in `cGPU`
- Copy `cGPU` to `c`
- Compute the execution time
- Free the GPU memory using `cudaFree`

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Global index

- `int idx = threadIdx.x + blockIdx.x*blockDim.x;` ensures coalesced access to global memory
- `int idx = threadIdx.x*gridDim.x + blockIdx.x;` is however a very bad choice
- The value of each `idx` is stored in a register

Registers

- Divided homogeneously between threads of the same block
- Have a lifetime of a kernel
- Cannot be used for arrays

Unified Memory A single virtual address space accessible from the host and any device

- The double allocation using `malloc` and `cudaMalloc` can be replaced by `cudaMallocManaged`
- `cudaDeviceSynchronize` is needed to make the CPU wait for GPU before accessing the data
- Page table entries may not be created until they are accessed. The pages can migrate to any processor's memory at any time
- Unified memory is very beneficial when there is an important movement of data especially between the CPU and GPU
- Unified memory is not a good option when the data stay in the same memory space
- Unified memory is necessary for enabling peer-to-peer transfer of data, directly across the PCIe bus or NVLink, bypassing host memory

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CPU timers
- Kernel launches and memory-copy functions are asynchronous, as are many CUDA API functions
- Necessary to synchronize by calling `cudaDeviceSynchronize` immediately before starting and stopping the CPU timer
- Used to time an overall solution that involves various kernel callings or that involves also the host

GPU timer
- Timing measures on the GPU and does not involve the operating system
- Best choice for local optimization, like the execution time of one kernel
- Timing is expressed in milliseconds

```
float TimeVar;
cudaEvent_t start, stop;
testCUDA(cudaEventCreate(&start));
testCUDA(cudaEventCreate(&stop));
testCUDA(cudaEventRecord(start,0));

/*********************************************************

To compute the execution time of this part of the code

*********************************************************/

testCUDA(cudaEventRecord(stop,0));
testCUDA(cudaEventSynchronize(stop));
testCUDA(cudaEventElapsedTime(&TimeVar, start, stop));
testCUDA(cudaEventDestroy(start));
testCUDA(cudaEventDestroy(stop));
```

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Pricing European $X = e^{-rT} f(S_T)$

$E(X) \approx \frac{X_1 + X_2 + ... + X_n}{n}$, using a family $\{X_i\}_{i \le n}$ of i.i.d $\sim X$

- **Strong law of large numbers**:

$$P\left(\lim_{n\to+\infty} \frac{X_1 + X_2 + ... + X_n}{n} = E(X)\right) = 1$$

- **Central limit theorem**: denoting $\epsilon_n = E(X) - \frac{X_1 + X_2 + ... + X_n}{n}$

$$\frac{\sqrt{n}}{\sigma}\epsilon_n \to G \sim \mathcal{N}(0,1)$$

- There is a 95% chance of having $|\epsilon_n| \le 1.96\frac{\sigma}{\sqrt{n}}$

Euler scheme for Black & Scholes model

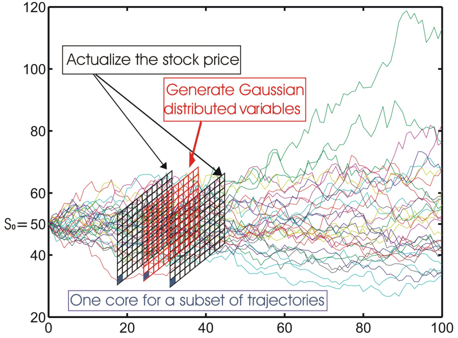
Given a time discretization sequence $t_k = kT/N$, with $k = 0, ..., N$ and $N = 100$, for $i = 1, ..., n$ we simulate

$$S^i_{t_k} = S^i_{t_{k-1}}\left[1 + rT/N + \sigma\sqrt{T/N}G^i_k\right], \quad S_0 = 50, \tag{1}$$

where the risk-free rate $r = 0.1$, the volatility $\sigma = 0.2$, and $(G^i_k)^{i=1,...,n}_{k=1,...,N}$ are independent normal random variables $\sim \mathcal{N}(0,1)$

Call Option

$f(x) = (x - K)_+ = \max(x - K, 0)$, with strike $K = S_0$ and maturity $T = 1$



For each time step $k < N$:

1 Random number generation (if parallelized) of G_k^i

2 Stock price actualization $S_{t_k}^i = S_{t_{k-1}}^i \left[1 + rT/N + \sigma\sqrt{T/N}G_k^i\right]$

Final time step $k = N$:

3 Compute the payoff $X^i = e^{-rT} f(S_T^i) = e^{-rT}(S_T^i - K)_+$

4 Send the values $(X^i)^{i=1,\dots,n}$ to the CPU for the approximation $E(X) \approx \dfrac{X_1 + X_2 + \dots + X_n}{n}$

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General Form of linear RNGs

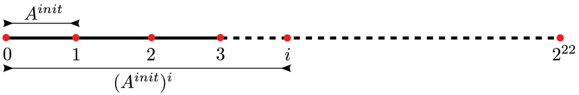
Without loss of generality:

$$X_n = (AX_{n-1} + C)\ mod(m) = (A\ :\ C)\begin{pmatrix} X_{n-1} \\ \dots \\ 1 \end{pmatrix}\ mod(m) \qquad (2)$$

Parallel-RNG from Period Splitting of One RNG

* Pierre L'Ecuyer proposed a very efficient RNG (1996) which is a CMRG on 32 bits: Combination of two MRG with $lag = 3$ for each MRG.
* Very long period $\sim 2^{185}$

$$x_n = (a_1 x_{n-1} + a_2 x_{n-2} + a_3 x_{n-3}) mod(m)$$



Parallel-RNG from Parameterization of RNGs

* Same parallelization as SPRNG Prime Modulus LCG.
* The same RNG with different parameters "a":

$$x_n = a x_{n-1} + c \quad mod(m)$$

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Black & Scholes PDE

$$\frac{\partial F}{\partial t}(t,x) + rx\frac{\partial F}{\partial x}(t,x) + \frac{1}{2}\sigma^2 x^2 \frac{\partial^2 F}{\partial x^2}(t,x) = rF(t,x), \quad F(T,x) = f(x)$$

With $u(t,x) = e^{r(T-t)}F(t,e^x)$, we equivalently solve the PDE

$$\frac{1}{2}\sigma^2 \frac{\partial^2 u}{\partial x^2}(t,x) + \mu\frac{\partial u}{\partial x}(t,x) = -\frac{\partial u}{\partial t}(t,x), \quad \mu = r - \frac{\sigma^2}{2}, \quad u(T,x) = f(e^x)$$

Put example

- $f(e^x) = \max(K - e^x, 0)$ where K is the strike
- The two limit conditions will be set at $x_{min} = \ln(K/2)$ and $x_{max} = \ln(2K)$ assuming heuristically that for all $t \in [0, T]$

$$u(t, x_{min}) = \mathtt{pmin} = K/2 \quad \& \quad u(t, x_{max}) = \mathtt{pmax} = 0 \tag{4}$$

PDE discretization

- σ takes its value in $[0.1, 0.5]$
- The volatility discretization involves $\mathtt{NB} = 64$ cells
- The space discretization involves $\mathtt{NTPB} = 256$ cells
- The time discretization of $[0, T]$ involves $\mathtt{N} = 10000$ time steps

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PDE explicit discretization

$$u_{i,j} = p_u u_{i+1,j+1} + p_m u_{i+1,j} + p_d u_{i+1,j-1}, \;\; u_{i,j} = u(t_i, x_j), \;\; u(T,x) = f(e^x),$$
$$p_u = \frac{\sigma^2 \Delta t}{2\Delta x^2} + \frac{\mu \Delta t}{2\Delta x}, \quad p_m = 1 - \frac{\sigma^2 \Delta t}{\Delta x^2}, \quad p_d = \frac{\sigma^2 \Delta t}{2\Delta x^2} - \frac{\mu \Delta t}{2\Delta x}, \quad \mu = r - \frac{\sigma^2}{2}$$

PDE implicit discretization

$$u_{i+1,j} = q_u u_{i,j+1} + q_m u_{i,j} + q_d u_{i,j-1}, \quad u_{i,j} = u(t_i, x_j), \quad u(T,x) = f(e^x),$$
$$q_u = -\frac{\sigma^2 \Delta t}{2\Delta x^2} - \frac{\mu \Delta t}{2\Delta x}, \quad q_m = 1 + \frac{\sigma^2 \Delta t}{\Delta x^2}, \quad q_d = -\frac{\sigma^2 \Delta t}{2\Delta x^2} + \frac{\mu \Delta t}{2\Delta x}$$

Tridiagonal system

solved with Thomas algorithm

$$\begin{pmatrix} d_1 & c_1 & & & 0 \\ a_2 & d_2 & c_2 & & \\ & a_3 & d_3 & \ddots & \\ & & \ddots & \ddots & \ddots \\ & 0 & & \ddots & \ddots & c_{n-1} \\ & & & & a_n & d_n \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix} \qquad (7)$$

Forward phase

$$c'_1 = \frac{c_1}{d_1}, \; y'_1 = \frac{y_1}{d_1}, \; c'_i = \frac{c_i}{d_i - a_i c'_{i-1}}, \; y'_i = \frac{y_i - a_i y'_{i-1}}{d_i - a_i c'_{i-1}} \text{ when } i = 2, ..., n$$

Backward phase

$$x_n = y'_n, \; x_i = y'_i - c'_i x_{i+1} \text{ when } i = n-1, ..., 1$$

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```
for(int k=0; k<N; k++){
   for(int j=0; j<NB; j++){
      sig = sigmin + dsig*j;
      mu = r - 0.5f*sig*sig;
      pu = 0.5f*(sig*sig*dt/(dx*dx) + mu*dt/dx);
      pm = 1.0f - sig*sig*dt/(dx*dx);
      pd = 0.5f*(sig*sig*dt/(dx*dx) - mu*dt/dx);
      for(int i=0; i<NTPB; i++){
         u = i+1;
         m = i;
         d = i-1;
         if(i==0){
           buff[i] = pmin;
         }else{
             if(i==NTPB-1){
               buff[i] = pmax;
             }else{
               buff[i] = pu*CPUTab[0][j][u] + pm*CPUTab[0][j][m] +
                         pd*CPUTab[0][j][d];
             }
         }
      }
      for(int i=0; i<NTPB; i++){
         CPUTab[0][j][i] = buff[i];
      }
   }
}
```