Houches 2016 : 6th School
Computational Physics

GPU : the disruptive technology of 21th century

Little comparison between CPU, MIC, GPU

Emmanuel Quémener
A (human) generation before... A serial B film in 1984

- 1984: The Last Starfighter
  - 27 minutes of synthetic images
  - $2.25 \times 10^9$ operations per image
  - Use of Cray X-MP (130 kW)
  - 66 days (in fact, 1 year needed)

- 2016: on GTX 1080Ti (250 W)
  - 3.4 secondes
  - Comparison GTX1080Ti / Cray
    - Performance : $1,600,000$
    - Consommation ~ $900,000,000$
« The beginning of all things »

- « Nvidia Launches Tesla Personal Supercomputer »
- When: on 19/11/2008
- Where: sur Tom's Hardware
- What: a PCIe card C1060 PCIe with 240 cores
- How much: 933 Gflops SP (but 78 Gflops DP)
What position for GPUs ?
The others « accelerators »

• Accelerator or the old history of coprocessors...
  – 1980 : 8087 (on 8086/8088) for floating points operations
  – 1989: 80387 (on 80386) and the respect of IEEE 754
  – 1990 : 80486DX and the integration of FPU inside the CPU
  – 1997 : K6-3DNow ! & Pentium MMX : SIMD inside the CPU
  – 1999 : SSE functions and the birth of a long serie (SSE4 & AVX)

• When chips stand out from CPU
  – 1998 : DSP style TMS320C67x as tools
  – 2008: Cell inside the PS3, IBM inside Road Runner and Top1 of Top500

• Business of compilers & very accurate programming model
Why a GPU is so powerful? To construct 3D scene!

- 2 approaches:
  - Raytracing: PovRay
  - Shadering: 3 operations

- Raytracing:
  - Starting from the eye to the objects of scene

- Shadering
  - Model2World: vectorial objects placed in the scene
  - World2View: projection of objects on a plan of view
  - View2Projection: pixelisation of vectorial plan of view
Why a GPU is so powerful
Shadering & Matrix computing

- **Modele 2 World**: 3 matrix products
  - Rotation
  - Translation
  - Scaling

- **World 2 View**: 2 matrix products
  - Camera position
  - Direction de l'endroit pointé

- **View 2 Projection**
  - Pixellisation

- **A GPU**: a « huge » Matrix Multiplier
How a GPU must be considered
A laboratory of parallelism

• You’ve got dozens of thousands of Equivalent PU!

• You have the choice between: CPU MIC GPU
How many elements inside?
Difference between GPU & CPU

- Operations
  - Matrix Multiply
  - Vectorization
  - Pipelining
  - Shader (multi)processor

- Programmation : 1993
  - OpenGL, Glide, Direct3D,

- Généricité : 2002
  - CgToolkit, CUDA, OpenCL
Why GPU is so powerful?
Come back generic processing

Inside the GPU

- Specialized processing units
- Pipelining efficiency

Adaptation Loss

- Changing scenes
- Different nature of details

The Solution
More generalist processing units!
Why is GPU so powerful
All « M » Flynn taxonomy included

• Vectorial : SIMD (Simple Instruction Multiple Data)
  – Addition of 2 positions (x,y,z) : 1 uniq command

• Parallel : MIMD (Multiple Instructions Multiple Data)
  – Several executions in parallel with the (almost) same data

• In fact, SIMT : Simple Instruction Multiple Threads
  – All processing units share the Threads
  – Each processing unit can work independently from others

• Need to the Threads
Important dates

- 1992-01 : OpenGL and the birth of a standard
- 1998-03 : OpenGL 1.2 and interesting functions
- 2002-12 : Cg Toolkit (Nvidia) and the extensions of language
  - Wrappers for all languages (Python)
- 2007-06 : CUDA (Nvidia) or the arrival of a real language
- 2008-06 : Snow Leopard (Apple) integrates OpenCL
  - La volonté d'utiliser au mieux sa machine ?
- 2008-11 : OpenCL 1.0 and its first specifications
- 2011-04 : WebCL and its first version by Nokia
Who use OpenCL
As applications

- **OS : Apple in MacOSX**
- **« Big » applications :**
  - Libreoffice
  - Ffmpeg
- **Known applications**
  - Graphical ones : photoscan,
  - Scientific : OpenMM, Gromacs, Lammmps, Amber, ...
- **Hundreds of softwares, libraries ! But checking is essentiel...**
  - https://www.khronos.org/opencl/resources/opencl-applications-using-opencl
Why GPU is a disruptive technology

How to reshuffle the cards in Scientific Computing

• In a conference in February 2006, this...
  - x100 in 5 years

• Between 2000 and 2015
  - GeForce 2 Go/GTX 980Ti: from 286 to 2816000 MOperations/s: x10000
  - Classical CPU: x100
Just a reminder of yesterday
Parallel programming models

<table>
<thead>
<tr>
<th></th>
<th>Cluster</th>
<th>Node CPU</th>
<th>Node GPU</th>
<th>Node Nvidia</th>
<th>Accelerator</th>
</tr>
</thead>
<tbody>
<tr>
<td>MPI</td>
<td>Yes</td>
<td>Yes</td>
<td>No</td>
<td>No</td>
<td>Yes*</td>
</tr>
<tr>
<td>PVM</td>
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<td>No</td>
<td>No</td>
<td>Yes*</td>
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<tr>
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<td>No</td>
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<td>Yes*</td>
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<tr>
<td>Pthreads</td>
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<td>No</td>
<td>No</td>
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</tr>
<tr>
<td>OpenCL</td>
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<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>CUDA</td>
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<td>No</td>
<td>Yes</td>
<td>No</td>
</tr>
<tr>
<td>TBB</td>
<td>No</td>
<td>Yes</td>
<td>No</td>
<td>No</td>
<td>Yes*</td>
</tr>
</tbody>
</table>

- OpenCL is the most versatile one
- CUDA can ONLY be used with Nvidia GPUs
- Accelerator seems to be the most universal, but...
Act as integrator: do not reinvent the wheel!

Parallel programming libraries

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<tbody>
<tr>
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<td>BLACS MKL</td>
<td>OpenBLAS MKL</td>
<td>clBLAS</td>
<td>CuBLAS</td>
<td>OpenBLAS MKL</td>
</tr>
<tr>
<td>LAPACK</td>
<td>Scalapack MKL</td>
<td>Atlas MKL</td>
<td>clMAGMA</td>
<td>MAGMA</td>
<td>MagmaMIC</td>
</tr>
<tr>
<td>FFT</td>
<td>FFTw3</td>
<td>FFTw3</td>
<td>clFFT</td>
<td>CuFFT</td>
<td>FFTw3</td>
</tr>
</tbody>
</table>

- Classic libraries can be used under GPU
  - Nvidia provides lots of implementations
  - OpenCL provides several on them, but not so complete
BLAS match : CPU vs GPU

xGEMM when x=D(P) or S(P)
Why OpenCL
Non Politically Correct History

• In the middle of 2000, Apple needs power for MacOSX
  – Some processing can be done by Nvidia chipsets
  – CUDA exists as a good successor of CgToolkit

• But Apple did not want to be jailed (as their users :-) )

• Apple promotes the Khronos consortium
  – AMD, IBM, ARM,
  – ... and Nvidia & Intel
What OpenCL offers
10 implementations on x86

• 3 implementations for CPU:
  – AMD one: the original
  – Intel one: efficient for specific parallel rate
  – PortableCL (POCL): OpenSource

• 3 implementations for GPU:
  – AMD one: for AMD/ATI graphical boards
  – Nvidia one: for Nvidia graphical boards
  – « Beignet » one: Open Source one for Intel Graphical Chipset

• 1 implementation for Accelerator:
  – Intel one: for Xeon Phi

• On other platforms, it seems to be possible
Goal: replace loop by distribute 2 types of distributions

• Blocks/WorkItems
  – Domain « global », large but slow amount of memory available

• Threads
  – Domain « local », small but quick amount of memory available
  – Needed for synchronisation of process

• Different access to memory:

• « clinfo » to get the properties of CL devices: Max work items
  – Max work items: 1024x1024x1024 for CPU so 1 billion distribution
How?
A « Hello World » in OpenCL...

- Define two vectors in ASCII
- Duplicate them in 2 huge vectors
- Add them using a OpenCL kernel
- Définir deux vecteurs en « Ascii »
- Print them on screen

Add of 2 vectors $a + b = c$
For each $n$:
$c[n] = a[n] + b[n]$
Differences between CUDA/OpenCL

```c
__device__ ulong MainLoop(ulong iterations, uint seed_w, uint seed_z, size_t work)
{
    uint jcong=seed_z+work;
    ulong total=0;
    for (ulong i=0; i<iterations; i++) {
        float x=CONGfp;
        float y=CONGfp;
        ulong inside=((x*x+y*y) <= THEONE) ? 1:0;
        total+=inside;
    }
    return(total);
}
__global__ void MainLoopBlocks(ulong *s, ulong iterations, uint seed_w, uint seed_z)
{
    ulong total=MainLoop(iterations, seed_z, seed_w, blockIdx.x);
    s[blockIdx.x]=total;
    __syncthreads();
}
__kernel void MainLoopGlobal(__global ulong *s, ulong iterations, uint seed_w, uint seed_z)
{
    ulong total=MainLoop(iterations, seed_z, seed_w, get_global_id(0));
    s[get_global_id(0)]=total;
    barrier(CLK_GLOBAL_MEM_FENCE);
}
```
Kernel Code & Build and Call

Add a vector in OpenCL

```c
__kernel void VectorAdd(__global int* c, __global int* a, __global int* b)
{
    // Index of the elements to add
    unsigned int n = get_global_id(0);
    // Sum the n-th element of vectors a and b and store in c
    c[n] = a[n] + b[n];
}
```

```python
OpenCLProgram = cl.Program(ctx, OpenCLSource).build()
OpenCLProgram.VectorAdd(queue, HostVector1.shape, None, GPUOutputVector, GPUVector1, GPUVector2)
```
How to OpenCL?

Write « Hello World! » in C

```c
#include <stdio.h>
#include <stdlib.h>
#include <CL/cl.h>

const char* OpenCLSource[] = {
    "__kernel void VectorAdd(__global int* c, __global int* a, __global int* b),",
    "{",
    "    // Index of the elements to add \n",
    "    unsigned int n = get_global_id(0);",
    "    // Sum the n'th element of vectors a and b and store in c \n",
    "    c[n] = a[n] + b[n];",
    "}"
};

int InitialData1[20] = {37, 50, 54, 56, 0, 43, 17, 71, 32, 36, 16, 43, 56, 100, 50, 25, 15, 17};
int InitialData2[20] = {35, 51, 54, 58, 55, 32, 36, 69, 27, 39, 35, 40, 16, 44, 55, 14, 58, 75, 18, 15};
#define SIZE 2048

int main(int argc, char **argv)
{
    int HostVector1[SIZE], HostVector2[SIZE];
    for(int c = 0; c < SIZE; c++)
    {
        HostVector1[c] = InitialData1[c%20];
        HostVector2[c] = InitialData2[c%20];
    }

    cl_platform_id cpPlatform;
    clGetPlatformIDs(1, &cpPlatform, NULL);
    cl_int ciErr1;
    cl_device_id cdDevice;
    clErr1 = clGetDeviceIDs(cpPlatform, CL_DEVICE_TYPE_GPU, 1, &cdDevice, NULL);
    cl_context GPUContext = clCreateContext(0, 1, &cdDevice, NULL, NULL, &ciErr1);
    cl_command_queue cqCommandQueue = clCreateCommandQueue(GPUContext, cdDevice, 0, NULL);
    cl_mem GPUVector1 = clCreateBuffer(GPUContext, CL_MEM_READ_ONLY | CL_MEM_COPY_HOST_PTR, sizeof(int) * SIZE, HostVector1, NULL);
    cl_mem GPUVector2 = clCreateBuffer(GPUContext, CL_MEM_READ_ONLY | CL_MEM_COPY_HOST_PTR, sizeof(int) * SIZE, HostVector2, NULL);
    cl_mem GPUOutputVector = clCreateBuffer(GPUContext, CL_MEM_WRITE_ONLY, sizeof(int) * SIZE, NULL, NULL);
    cl_program OpenCLProgram = clCreateProgramWithSource(GPUContext, 7, OpenCLSource, NULL, NULL);
    clBuildProgram(OpenCLProgram, 0, NULL, NULL, NULL, NULL);
    cl_kernel OpenCLVectorAdd = clCreateKernel(OpenCLProgram, "VectorAdd"), NULL);
    clSetKernelArg(OpenCLVectorAdd, 0, sizeof(cl_mem), (void*)&GPUOutputVector);
    clSetKernelArg(OpenCLVectorAdd, 1, sizeof(cl_mem), (void*)&GPUVector1);
    clSetKernelArg(OpenCLVectorAdd, 2, sizeof(cl_mem), (void*)&GPUVector2);
    size_t WorkSize[1] = {SIZE}; // one dimensional Range
    clEnqueueNDRangeKernel(cqCommandQueue, OpenCLVectorAdd, 1, NULL, WorkSize, NULL, 0, NULL, NULL);
    int HostOutputVector[SIZE];
    clEnqueueReadBuffer(cqCommandQueue, GPUOutputVector, CL_TRUE, 0, SIZE * sizeof(int), HostOutputVector, 0, NULL, NULL);
    clReleaseKernel(OpenCLVectorAdd);
    clReleaseProgram(OpenCLProgram);
    clReleaseCommandQueue(cqCommandQueue);
    clReleaseContext(GPUContext);
    clReleaseMemObject(GPUVector1);
    clReleaseMemObject(GPUVector2);
    clReleaseMemObject(GPUOutputVector);
    for (int Rows = 0; Rows < (SIZE/20); Rows++) {
        printf("\t");
        for(int c = 0; c <20; c++) {
            printf("%c", (char)HostOutputVector[Rows * 20 + c]);
        }
        printf("\n\nThe End\n\n"),
    return 0;
}
```

OpenCL kernel

Kernel Call

Number of lines Of OpenCL kernel
import pyopencl as cl
import numpy.linalg as la
import sys

OpenCLSource = ""

__kernel void VectorAdd(__global int* c, __global int* a, __global int* b)
{
    // Index of the elements to add
    unsigned int n = get_global_id(0);
    // Sum the n th element of vectors a and b and store in c
    c[n] = a[n] + b[n];
}

""

InitialData1=[37,50,54,50,56,0,43,43,74,71,32,36,16,43,56,100,50,25,15,17]
InitialData2=[35,51,54,58,55,32,36,69,27,39,35,40,16,44,55,14,58,75,18,15]

SIZE=2048

HostVector1=numpy.zeros(SIZE).astype(numpy.int32)
HostVector2=numpy.zeros(SIZE).astype(numpy.int32)

for c in range(SIZE):
    HostVector1[c] = InitialData1[c%20]
    HostVector2[c] = InitialData2[c%20]

ctx = cl.create_some_context()
queue = cl.CommandQueue(ctx)

mf = cl.mem_flags
GPUVector1 = cl.Buffer(ctx, mf.READ_ONLY | mf.COPY_HOST_PTR, hostbuf=HostVector1)
GPUVector2 = cl.Buffer(ctx, mf.READ_ONLY | mf.COPY_HOST_PTR, hostbuf=HostVector2)
GPUOutputVector = cl.Buffer(ctx, mf.WRITE_ONLY, HostVector1.nbytes)

OpenCLProgram = cl.Program(ctx, OpenCLSource).build()

OpenCLProgram.VectorAdd(queue, HostVector1.shape, None, GPUOutputVector, GPUVector1, GPUVector2)

HostOutputVector = numpy.empty_like(HostVector1)

cl.enqueue_copy(queue, HostOutputVector, GPUOutputVector)

GPUVector1.release()
GPUVector2.release()
GPUOutputVector.release()

OutputString=''

for rows in range(SIZE/20):
    OutputString+='\t'
    for c in range(20):
        OutputString+=chr(HostOutputVector[rows*20+c])

print OutputString
sys.stdout.write("\nThe End\n\n");
You think Python is not efficient? Let’s have a quick comparison...

![Comparison chart showing performance of different configurations: MPI+C, MPI+OpenMP/C, MPI+PyOpenCL NoHT, MPI+PyOpenCL HT.](chart.png)
Pi Dart Board match (yesterday) : Python vs C & CPU vs GPU vs Phi

2 Chips on Board !
How to OpenCL?
« Hello World » C/Python : to weight

• On previous OpenCL implementations :
  – In C : 75 lines, 262 words, 2848 bytes
  – In Python : 51 lines, 137 words, 1551 bytes
  – Factors : 0.68, 0.52, 0.54 in lines, words and bytes.

• Programming OpenCL :
  – Difficult programming context
    • « To open the box in more difficult than to assemble the furniture unit ! »
    • Requirement to simplify the calls by an API
  – No compatibility between SDK of AMD and Nvidia
    • Everyone rewrite their own API

• One solution, however « The » solution : Python
Small comparison between *PU MIC Phi emerges, GPU ambushed

From 1 to 1024 PR
Deep exploration of Parallel Rates
Parallel Rate from 1024 to 16384

PR from 1024 to 16384

Comparaison sur Pi Monte Carlo en OpenCL

Comparaison sur Pi Monte Carlo en OpenCL

All prime numbers > 1024.

Emmanuel QUÉMENER CC BY-NC-SA
June 2, 2016
Deep exploration of Parallel Rates
Parallel Rate from 1024 to 65536

AMD HD7970 & R9-290
Long Period : 4x number of ALU

Nvidia GTX Titan & Tesla K40
Short Period : number of SMX units

Period of 14
(14 SMX)

Period of 15
(15 SMX)
Splutter code on OpenCL devices

Splutter sur 16 MB en OpenCL

- Intel IvyBridge & Haswell
- Accelerator Xeon Phi
- GPU AMD/ATI HD 7970 & R290X
- GPU Nvidia GT, GTX, Tesla
Behaviour of 20 (GP)GPU vs PR
Is Parallel Envelop reproducible ?
For 2 specific boards...

Nvidia GT620
AMD HD6450
Variability: A distinctive criterion! What a strange property :-/ ...
Inside your VirtualBox OpenCL CPU implementations

- What’s inside :
  - The 3 CPU implementations for OpenCL: AMD, Intel and Open Source

- How to get OpenCL devices?
  - clinfo

- How to launch a small example in Python
  - python /usr/share/doc/python-pyopencl-doc/examples/benchmark.py

- How to launch my test codes:
What does it look like?
Let's have a look to the codes!

- MPI implementation in C
- MPI+OpenMP implementation in C
- OpenCL implementation in Python
- Threads+OpenCL implementation in Python
- MPI+OpenCL implementation in Python
Conclusion

- Now, the « brute » power is inside the GPUs
- But, QPU (PR=1) of GPU is 50x slower than CPU
- To exploit GPU, parallel rate MUST be over 1000
- To program GPU, prefer :
  - Developer approach : Python with PyOpenCL (or PyCUDA)
  - Integrator approach : external libraries optimized
- In all cases, instrument your launches!