Houches 2016 : 6th School

Computational Physics

GPU : the disruptive technology of 21th century

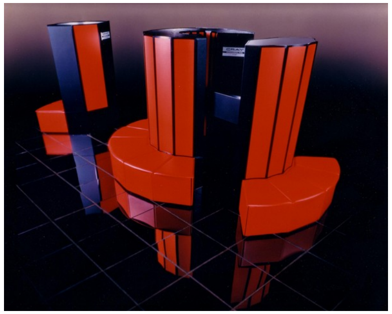
Little comparison between CPU, MIC, GPU

Emmanuel Quémener

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

- 1984 : The Last Starfighter
  - 27 minutes of synthetic images
  - 22.5 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 !



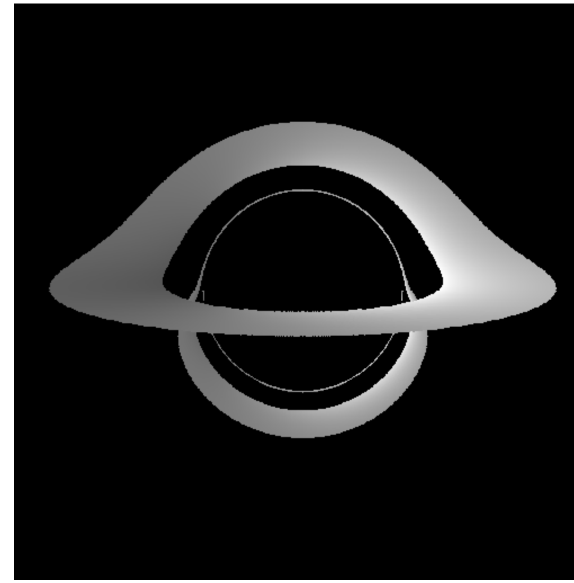
« The beginning of all things »

- « Nvidia Launches Tesla Personal Supercomputer »
- When : on 19/11/2008 Qui : Nvidia
- 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

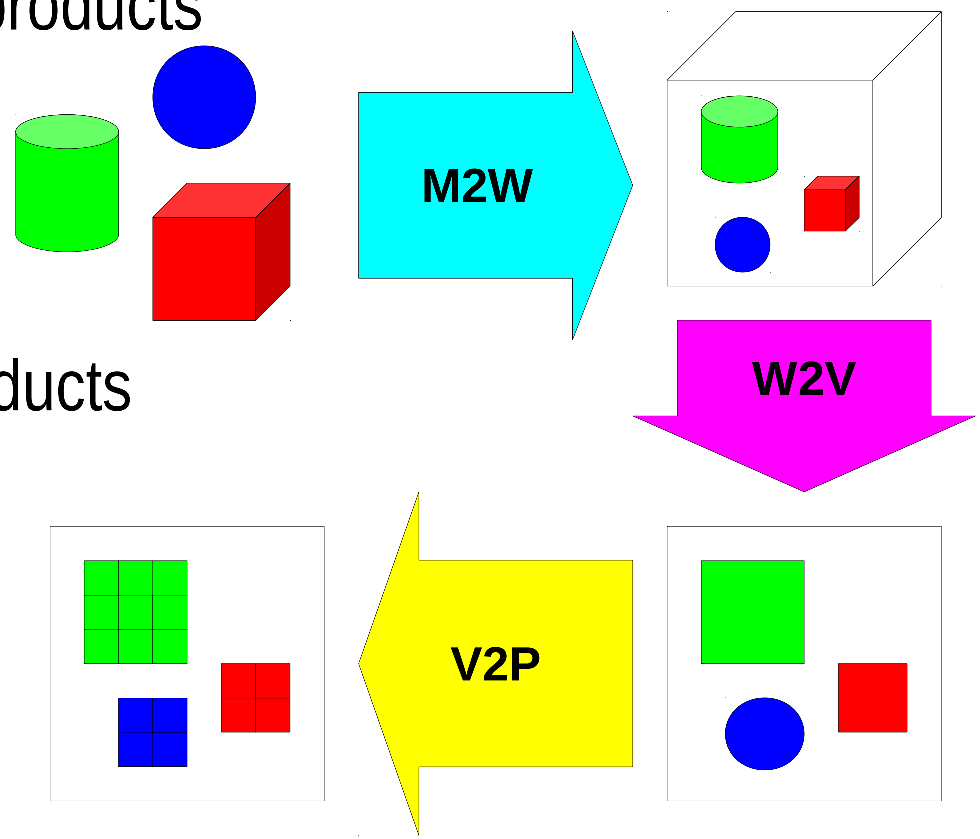
Why a GPU is so powerful ? To construct 3D scene !



- 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

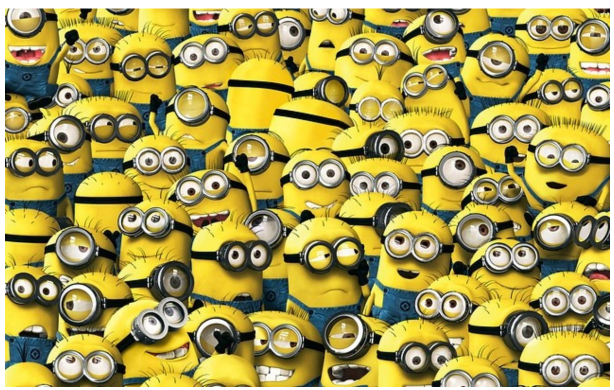
Why a GPU is so powerful Shadering & Matrix computing

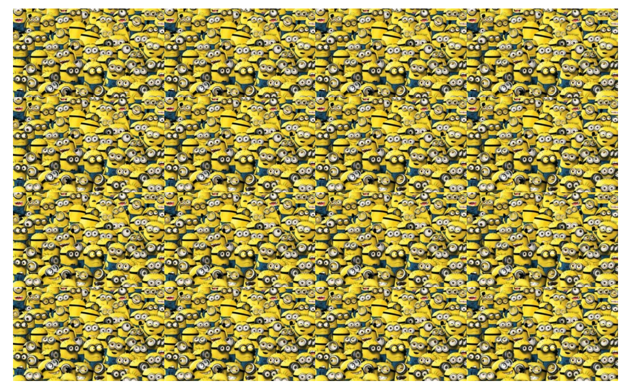
- **Modele 2 World** : 3 matrix products
  - Rotation
  - Translation
  - Scaling
- **World 2 View** : 2 matrix products
  - Camera position
  - Direction de l'endroit pointé
- **View 2 Projection**
  - Pixellisation
- A GPU : a « huge » Matrix Multiplier



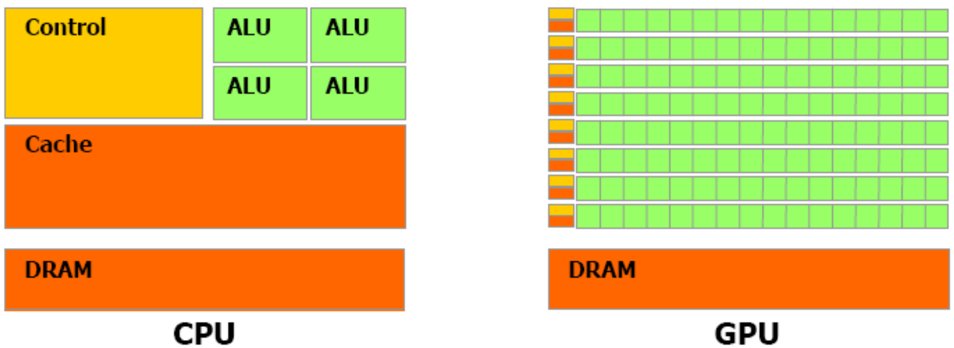
How a GPU must be considered
A laboratory of parallelism

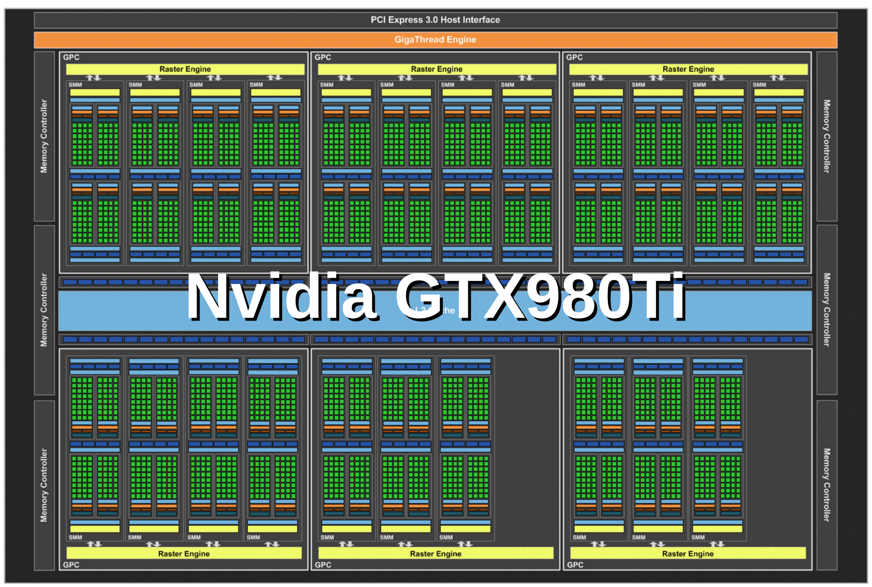
- You’ve got dozen of thousands of Equivalent PU !
- You have the choice between : **CPU MIC GPU**





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

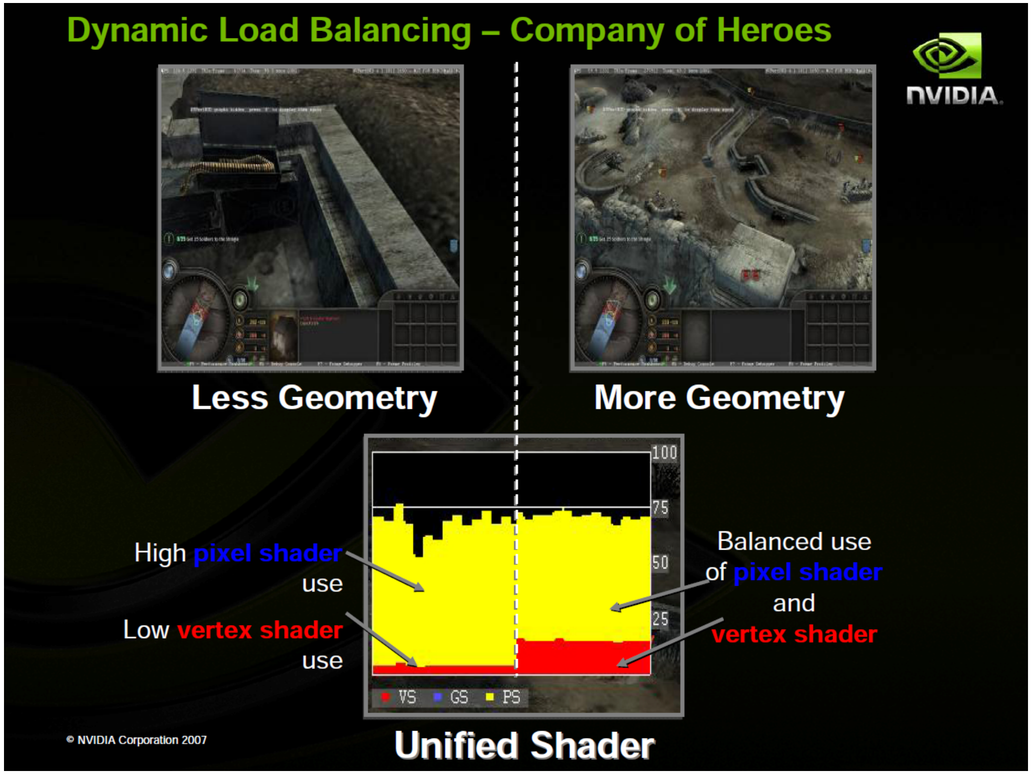
Why GPU is so powerful ? Come back generic processing

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 langague
- 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

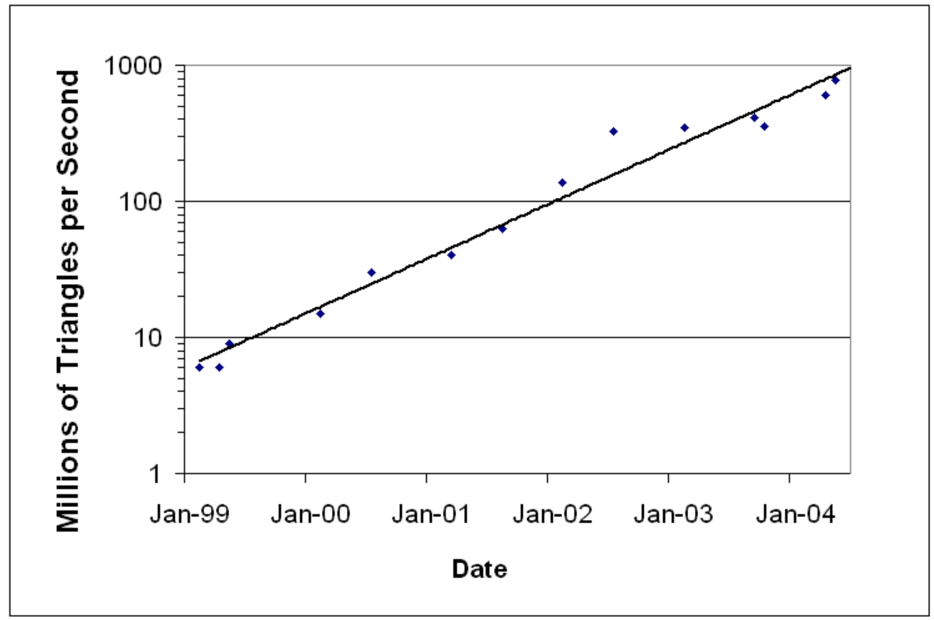
Who use OpenCL As applications

- OS : Apple in MacOSX
- « Big » applications :
  - Libreoffice
  - Ffmpeg
- Known applications
  - Graphical ones : photoscan,
  - Scientific : OpenMM, Gromacs, Lammps, 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 remind of yesterday

Parallel programming models

	Cluster	**Node CPU**	Node GPU	Node Nvidia	Accelerator
MPI	Yes	Yes	No	No	Yes*
PVM	Yes	Yes	No	No	Yes*
OpenMP	No	Yes	No	No	Yes*
Pthreads	No	Yes	No	No	Yes*
OpenCL	No	Yes	Yes	Yes	Yes
CUDA	No	No	No	Yes	No
TBB	No	Yes	No	No	Yes*

- OpenCL is the most versatile one
- CUDA can ONLY be used with Nvidia GPUs
- Accelerator seems to be the most universal, but...

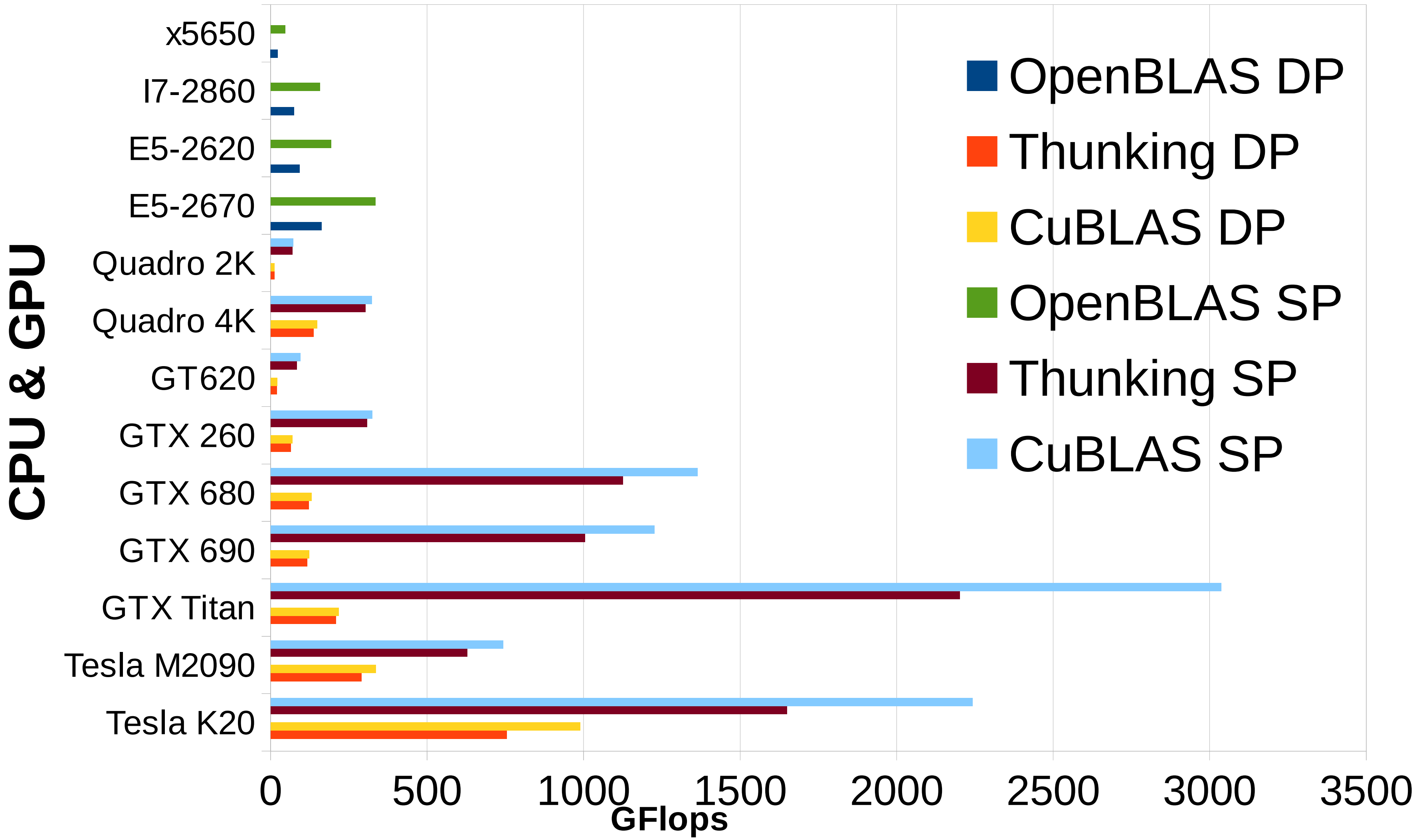
Act as integrator : do not reinvent the wheel !

Parallel programming librairies

	Cluster	**Node CPU**	Node GPU	Node Nvidia	Accelerator
BLAS	BLACS MKL	OpenBLAS MKL	clBLAS	CuBLAS	OpenBLAS MKL
LAPACK	Scalapack MKL	Atlas MKL	clMAGMA	MAGMA	MagmaMIC
FFT	FFTw3	FFTw3	clFFT	CuFFT	FFTw3

- Classic librairies 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]

Hello OpenCL World!	Hello OpenCL World!	Hello OpenCL World!	Hello OpenCL World!	Hello OpenCL World!	Hello OpenCL World!	Hello OpenCL World!	Hello OpenCL World!
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Differences between CUDA/OpenCL

```
__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;
  }
__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();
}
```

```
ulong MainLoop(ulong iterations,uint seed_z,uint seed_w,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);
}
__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));
  barrier(CLK_GLOBAL_MEM_FENCE);
  s[get_global_id(0)]=total;
}
```

Kernel Code & Build and Call Add a vector in OpenCL

```
__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];
}
```

```
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] = {37,50,54,50,56,0,43,43,74,71,32,36,16,43,56,100,50,25,15,17};
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;
  ciErr1 = 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

How to OpenCL ? Write « Hello World ! » in Python

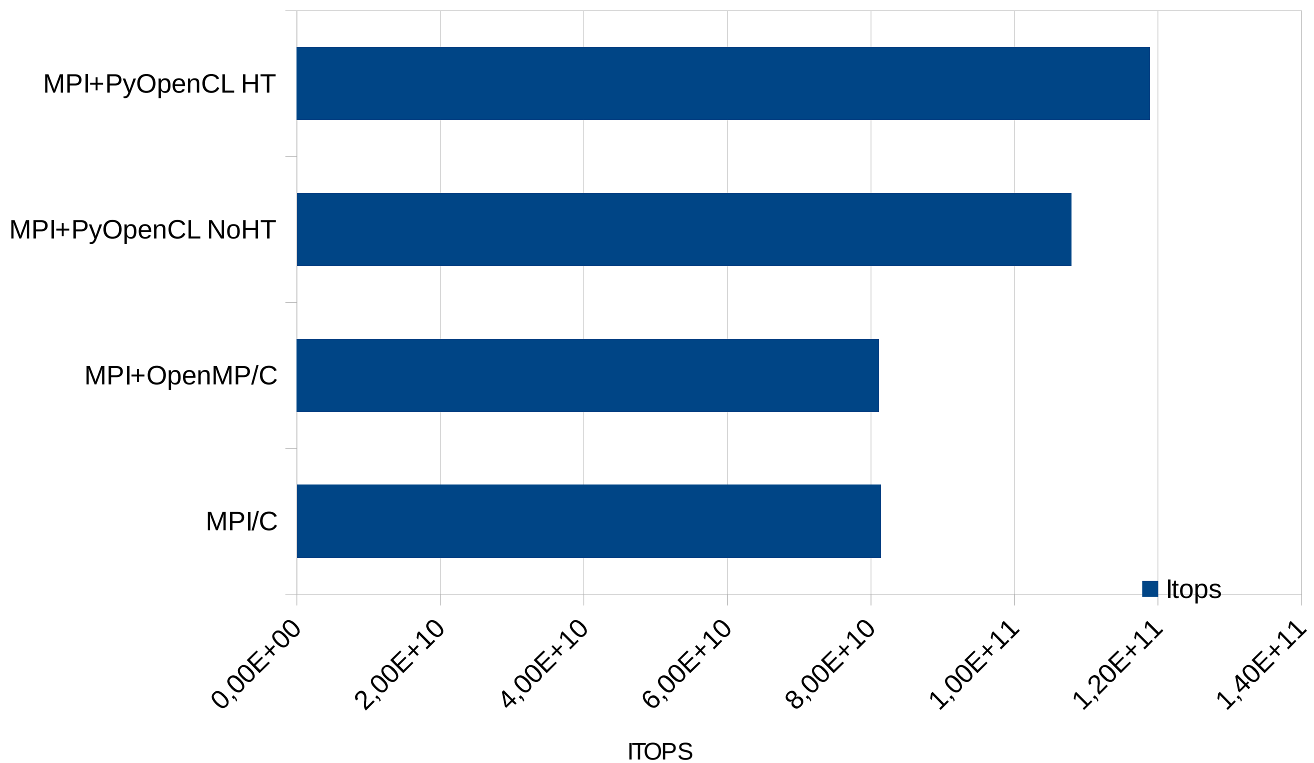
OpenCL kernel

```python
import pyopencl as cl
import numpy
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)
```

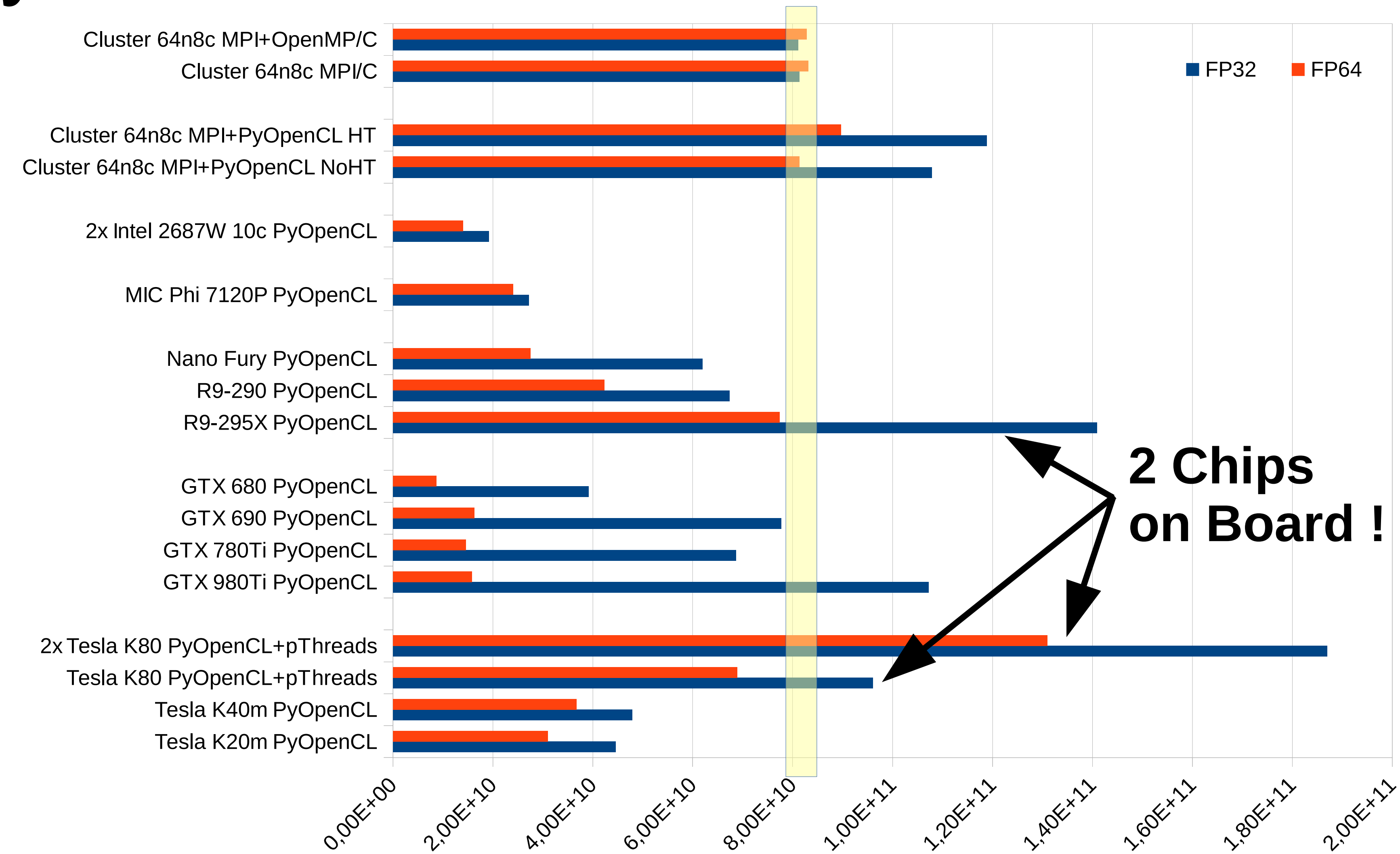
```python
mf = cl.mem_flags
GPUVector1 = cl.Buffer(ctx, mf.READ_ONLY | mf.COPY_HOST_PTR, hostbuf=HostVector1)
GPUVector2 = cl.Buffer(ctx, mf.READ_ONLY | mf.COPY_HOST_PTR, hostbuf=HostVector2)
GPUOutputVector = cl.Buffer(ctx, mf.WRITE_ONLY, HostVector1.nbytes)
OpenCLProgram = cl.Program(ctx, OpenCLSource).build()
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");
```

Kernel Call

You think Python is not efficient ? Let's have a quick comparison...



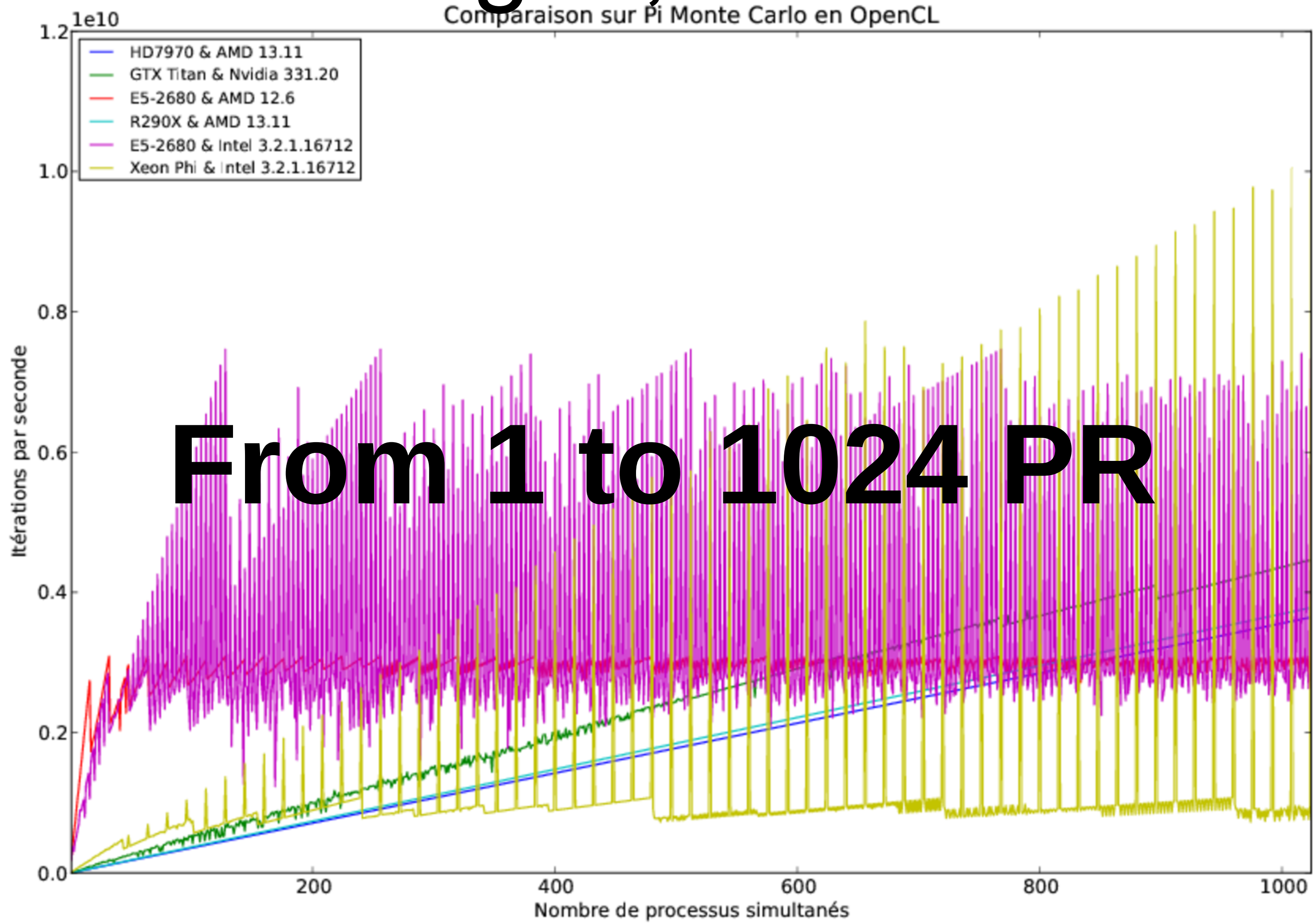
Pi Dart Board match (yesterday) : Python vs C & CPU vs GPU vs Phi



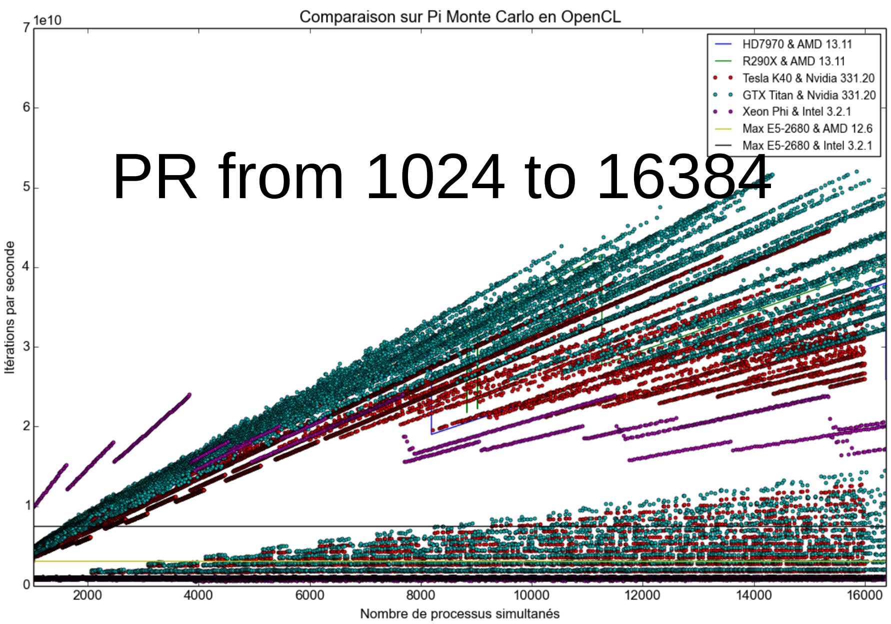
How to OpenCL ?
« Hello World » C/Python : to weight

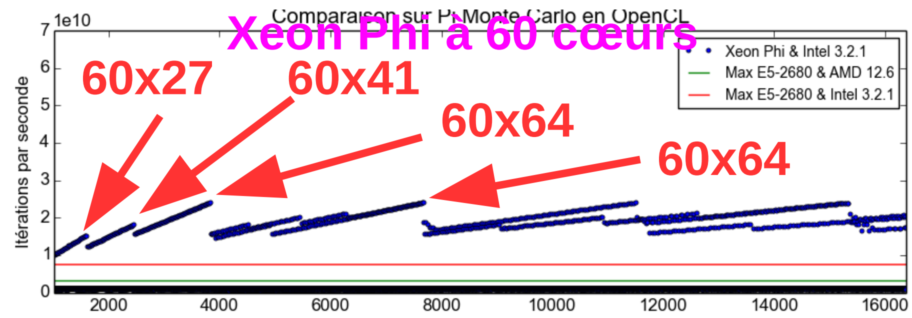
- On previous OpenCL implementations :
  - In C : 75 lines, 262 words, 2848 bytes
  - In Python : 51 lines, 137 words, 1551 bytes
  - Factors : 0.68, 0.52, 0.54 in lines, words and bytes.
- Programming OpenCL :
  - Difficult programming context
    - « To open the box in more difficult than to assemble 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

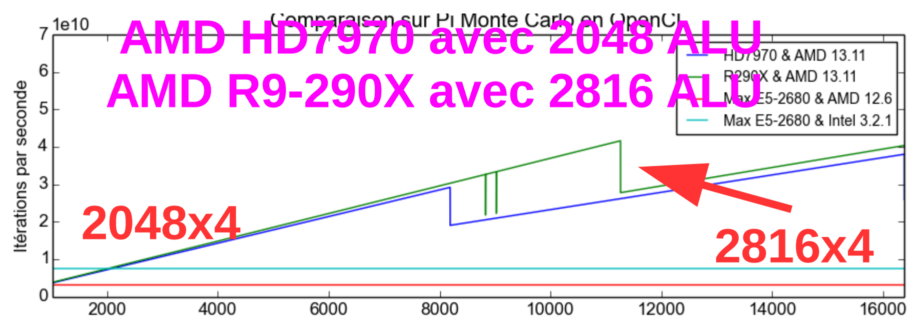
Small comparison between *PU
MIC Phi emerges, GPU ambushed

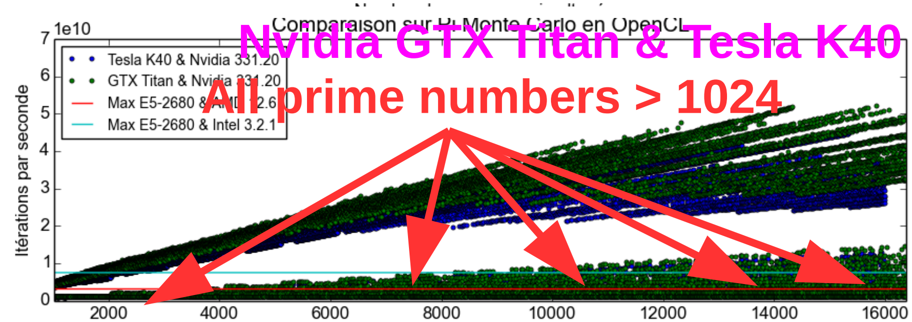


Deep exploration of Parallel Rates
Parallel Rate from 1024 to 16384

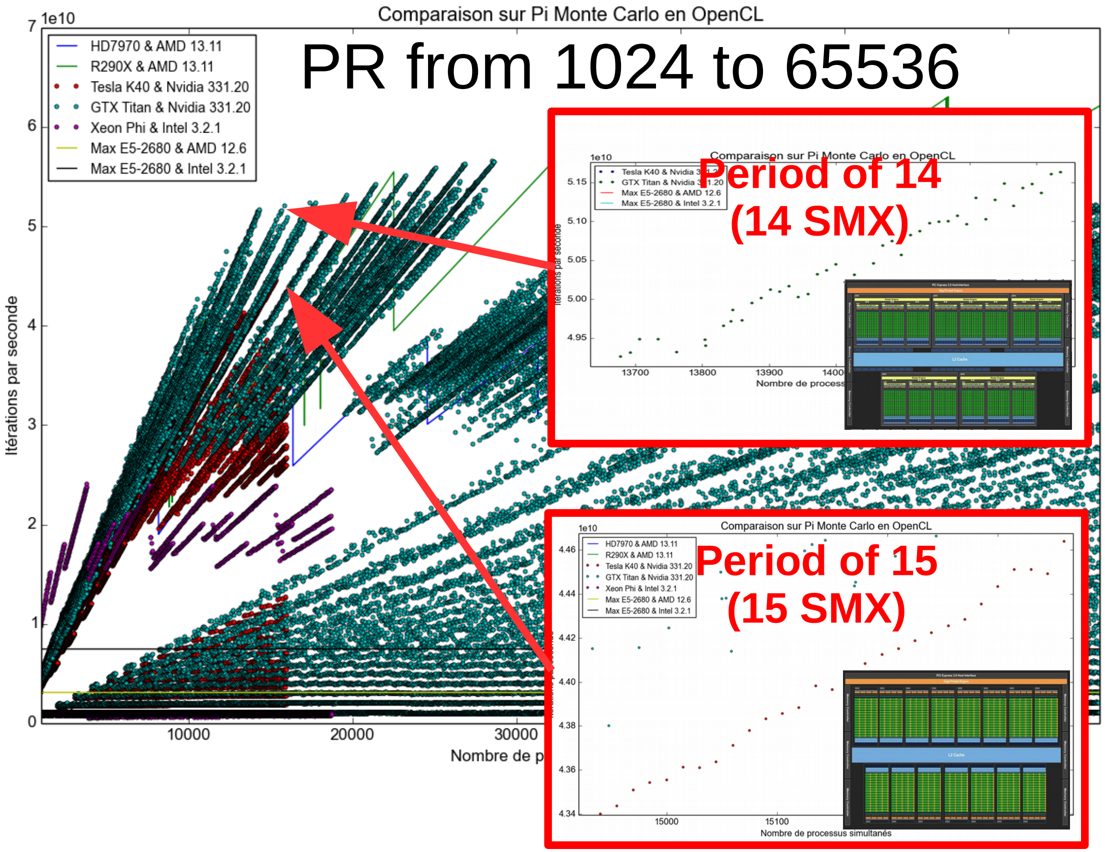




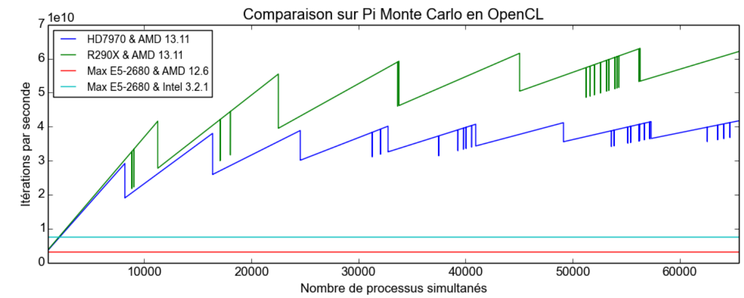




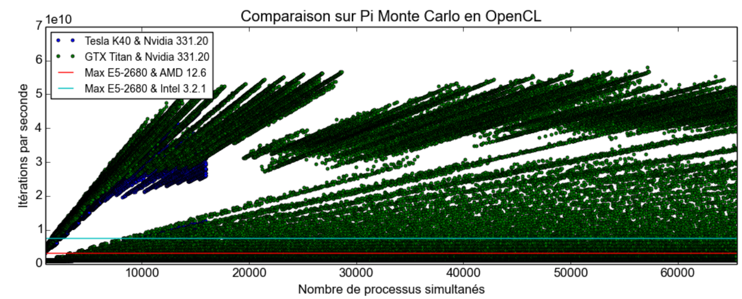
Deep exploration of Parallel Rates
Parallel Rate from 1024 to 65536



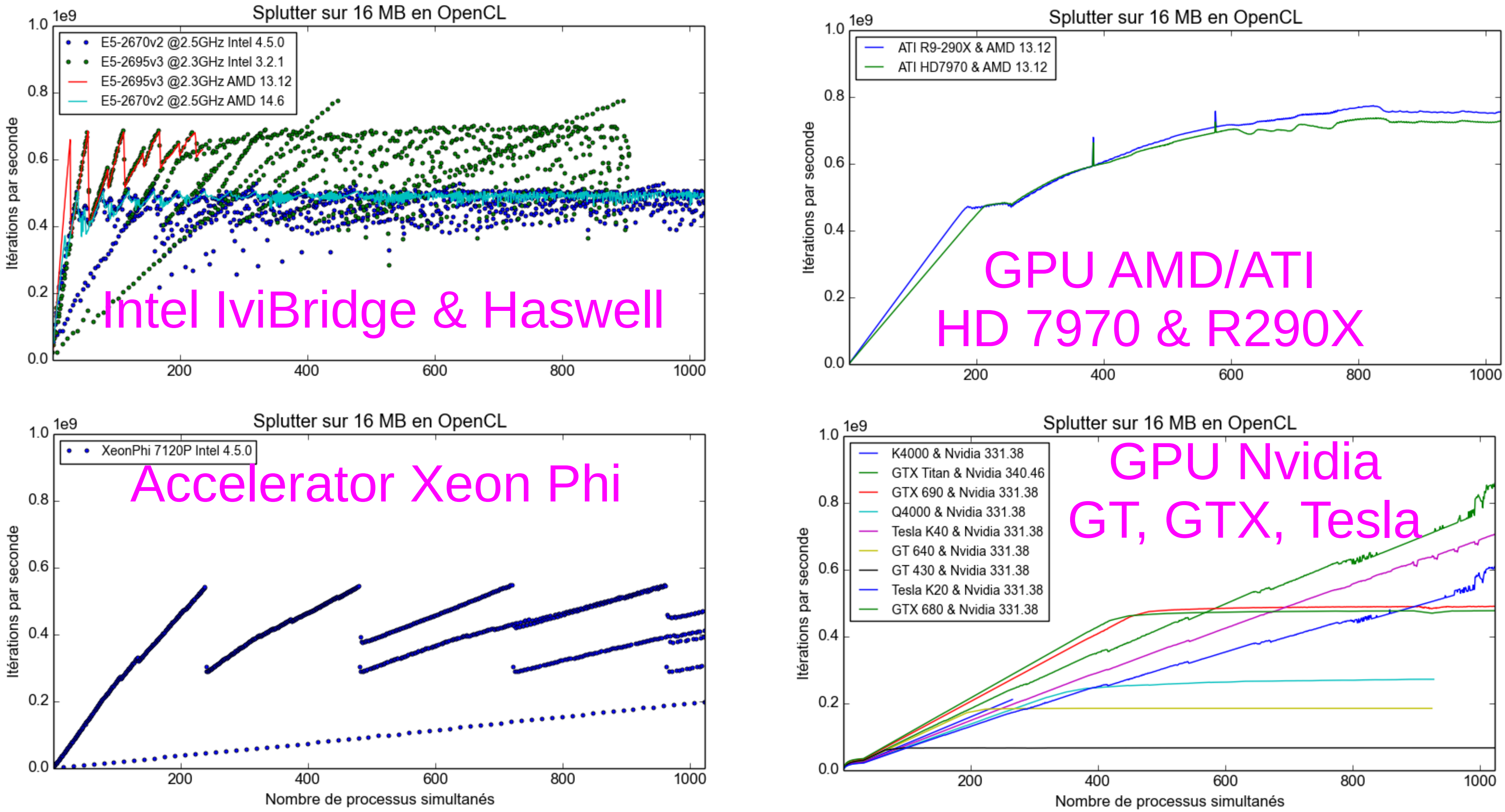
AMD HD7970 & R9-290
Long Period : 4x number of ALU



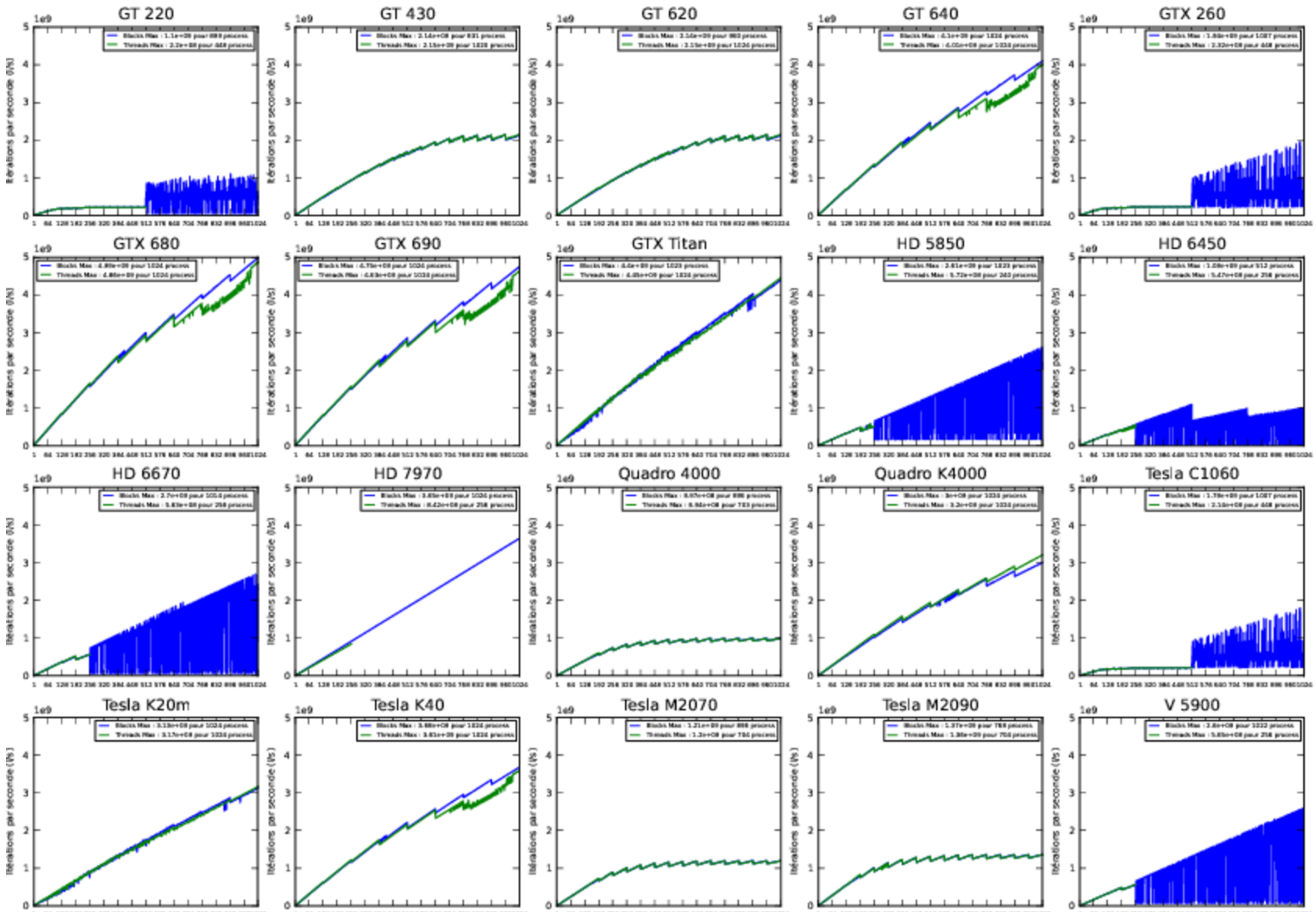
Nvidia GTX Titan & Tesla K40
Short Period : number of SMX units



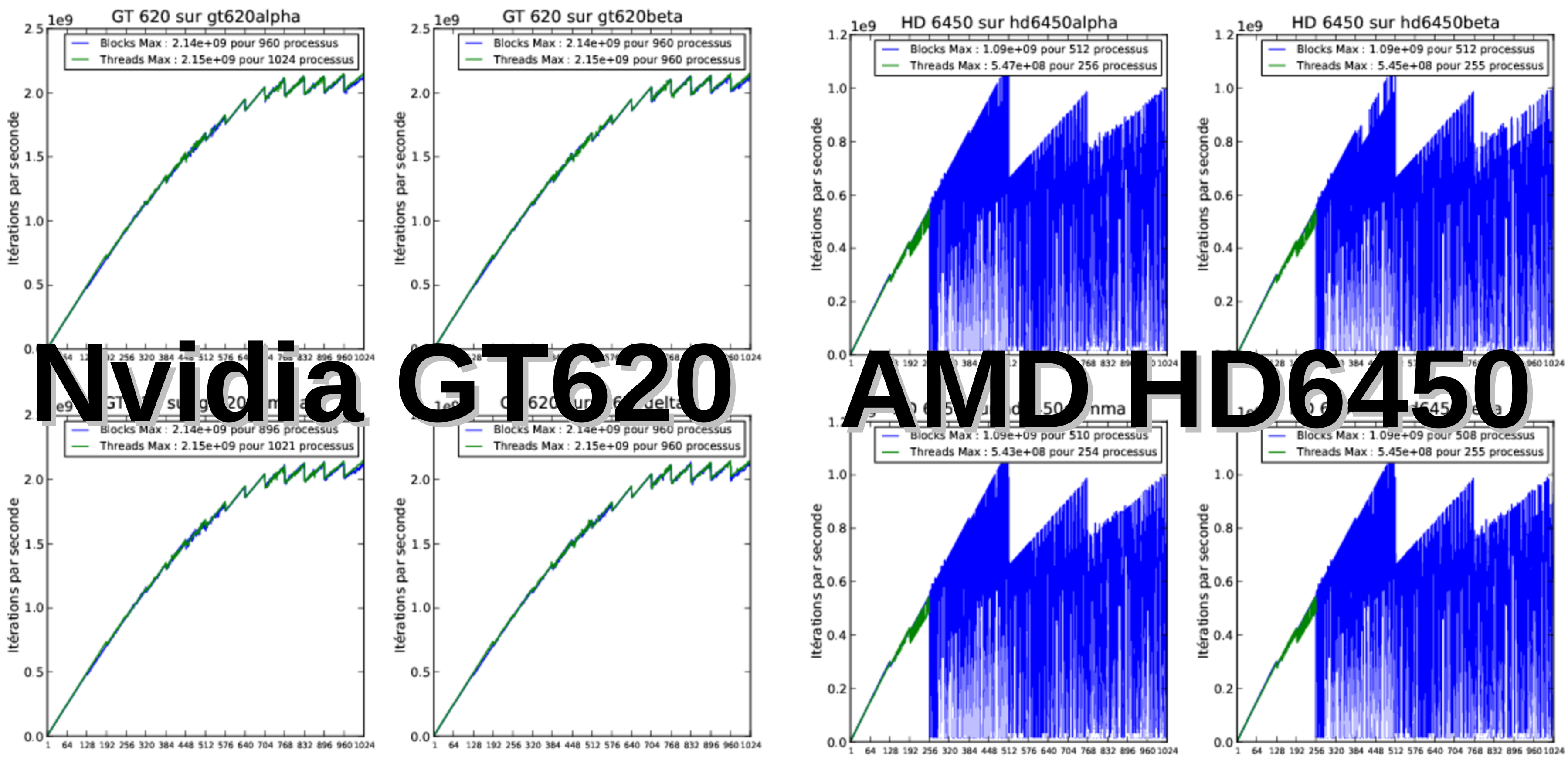
Splutter code on OpenCL devices



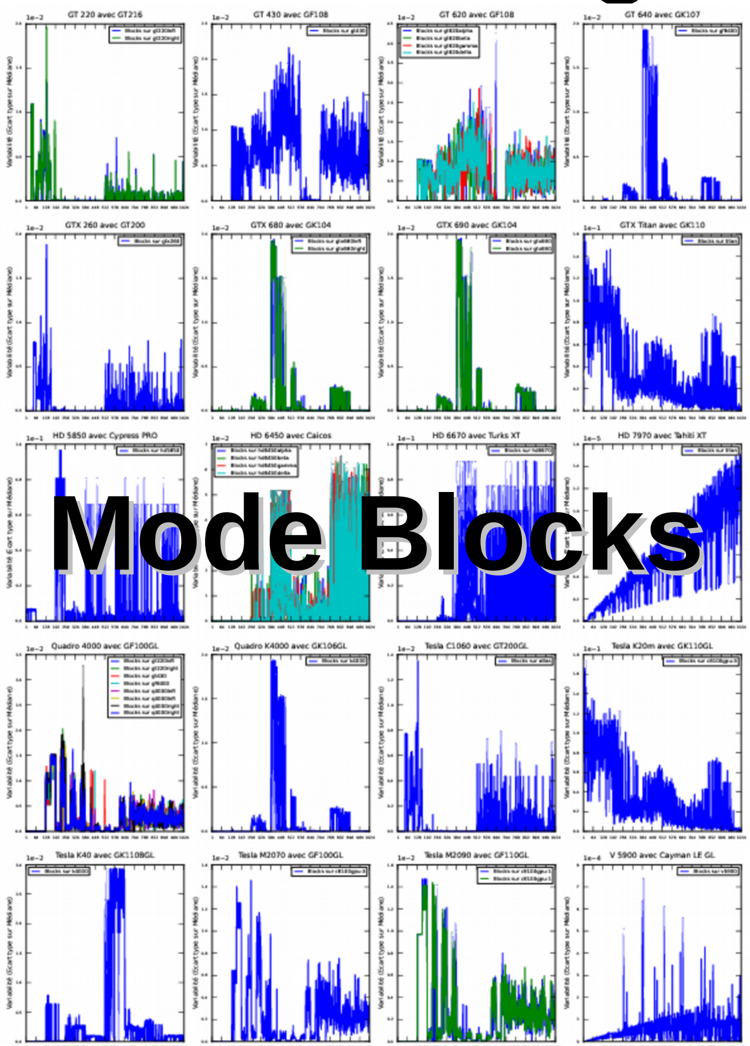
Behaviour of 20 (GP)GPU vs PR

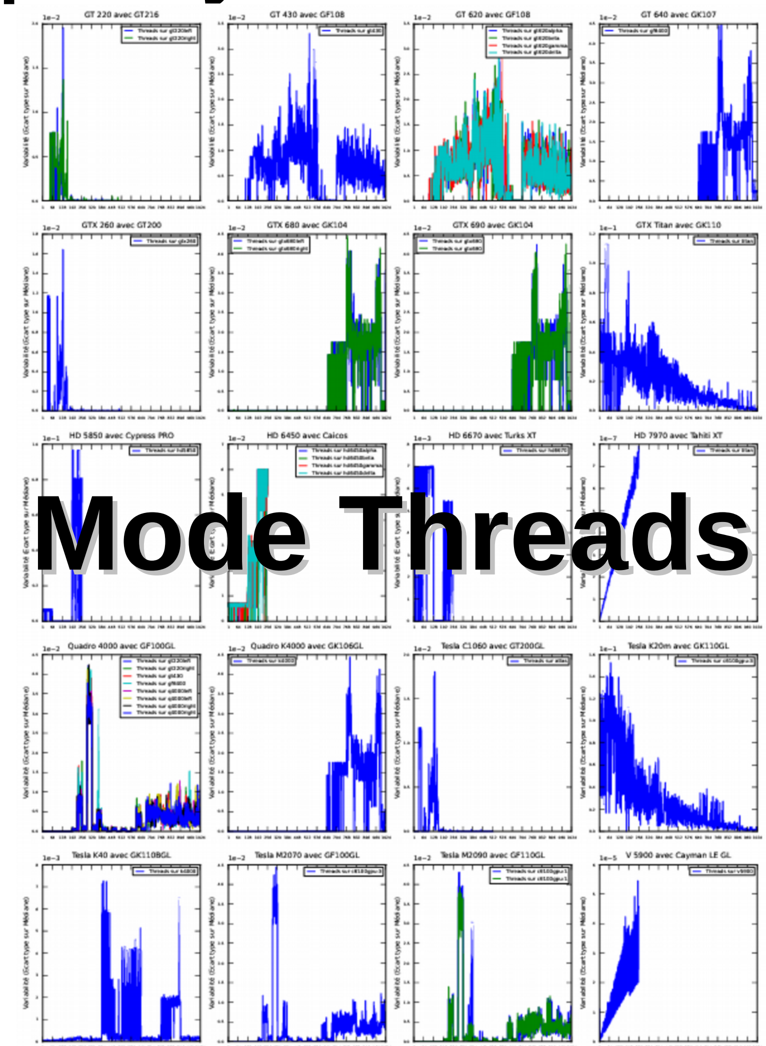


Is Parallel Envelop reproducible ? For 2 specific boards...



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/benckmark.py
- How to launch my test codes :
  - http://houches2016.no-ip.org/redmine/projects/parallelism/documents

What does it look like ?
Lets 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 !