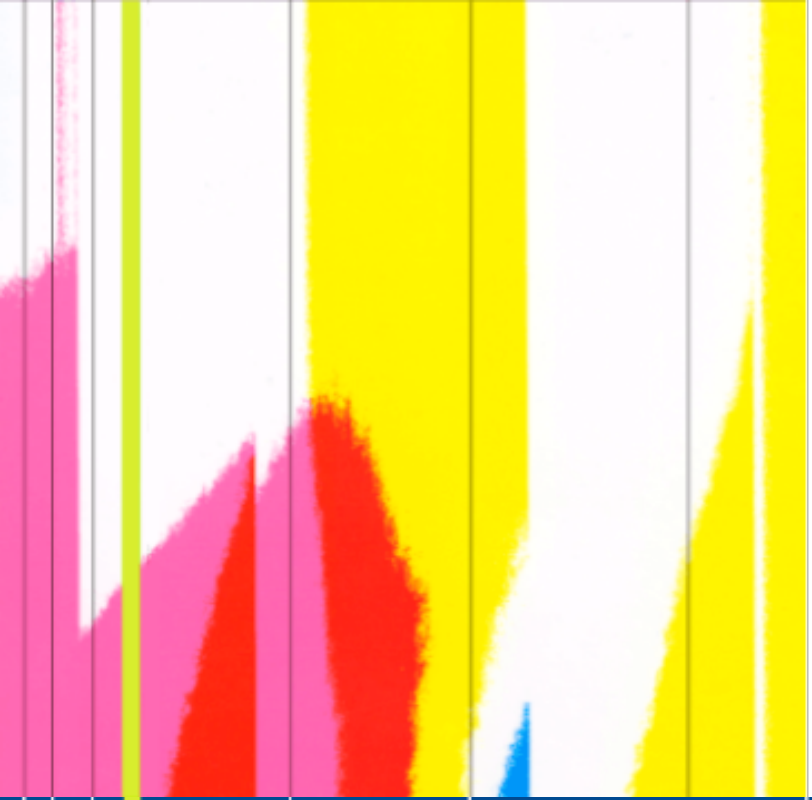

GPU for Dummies

Cédric Castagnède - François Rué
7 juin 2011

INSTITUT NATIONAL
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Outline

- CPU versus GPU: deep differences
  - CPU Architecture
  - GPU Architecture (NVIDIA Card)
  - We need new programming language... again...

- CUDA: an API with new concepts
  - Grid and blocs
  - Memory space overview
  - The useful functions
  - Extensions and Kernels
  - Difference between CUDA C and Fortran

Outline

- Why make it simple when it can be complicated?
  - Example 1: Transpose matrix
  - Several implementations
  - Example 2:Matrix multiplication
  - Several implementations

- Help me! Where are the libraries?
  - Libraries for CUDA?
  - Do not you see BLAS right there?
  - CUBLAS help to find performance
  - Outcome of all these sheets

Outline

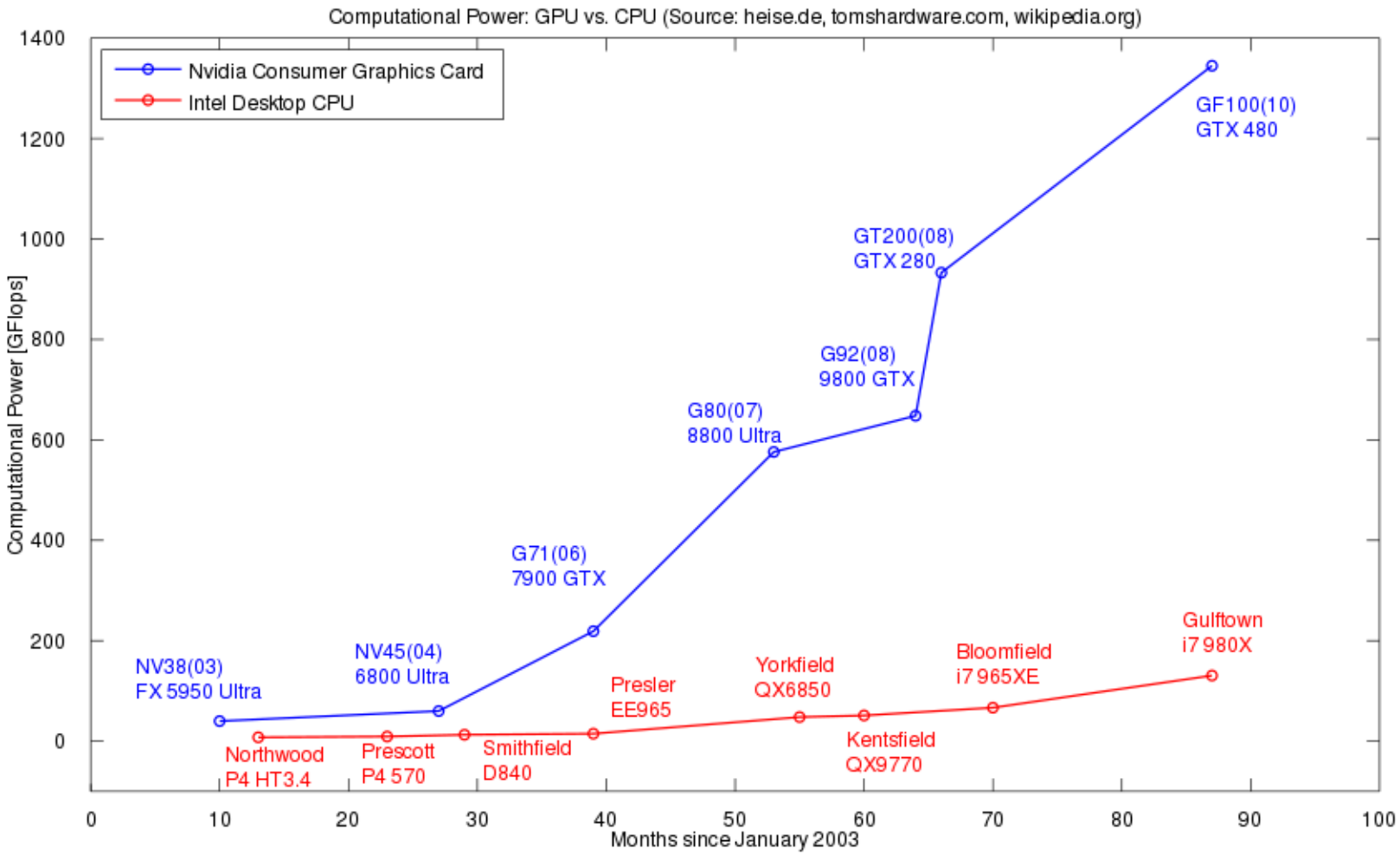
- And in real life...
  - You have a CPU implementation
  - Find out where you can place libraries calls
  - What we need to run on GPU
  - Outline

- Outlines
  - When going on GPU is profitable?
  - Go on GPU at your speed
  - Your implementation will be portable?
  - What is your future?

Why use GPU?

Because...

- GPU is very popular
  - thanks to video game
  - attractive market
- GPU are massively parallel
  - large local memory
  - high bandwidth memory
  - lot of cores and ALU
- Bandwidth is very important
- GPU cards are massively produced, so cluster cost is reduced
- Energy Efficiency is over 6 Gflops / watts


Computational Power: GPU vs. CPU (Source: heise.de, tomshardware.com, wikipedia.org)
Nvidia Consumer Graphics Card
Intel Desktop CPU
Computational Power [GFlops]
Months since January 2003
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NV38(03)
FX 5950 Ultra
NV45(04)
6800 Ultra
G71(06)
7900 GTX
G80(07)
8800 Ultra
G92(08)
9800 GTX
GT200(08)
GTX 280
GF100(10)
GTX 480
Northwood
P4 HT3.4
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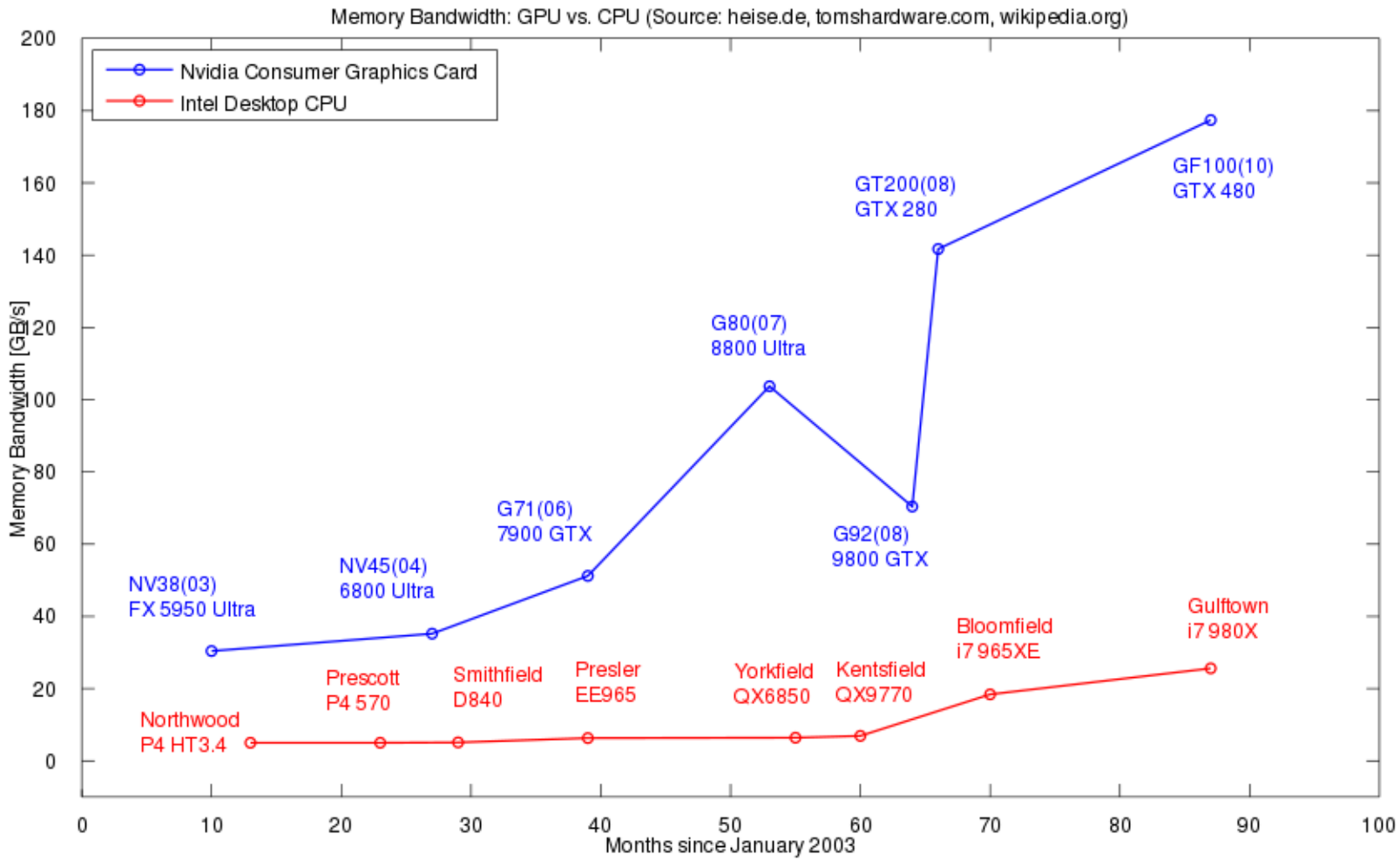
Gulftown
i7 980X


Memory Bandwidth: GPU vs. CPU (Source: heise.de, tomshardware.com, wikipedia.org)
Nvidia Consumer Graphics Card
Intel Desktop CPU
Memory Bandwidth [GB/s]
Months since January 2003
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6800 Ultra
G71(06)
7900 GTX
G80(07)
8800 Ultra
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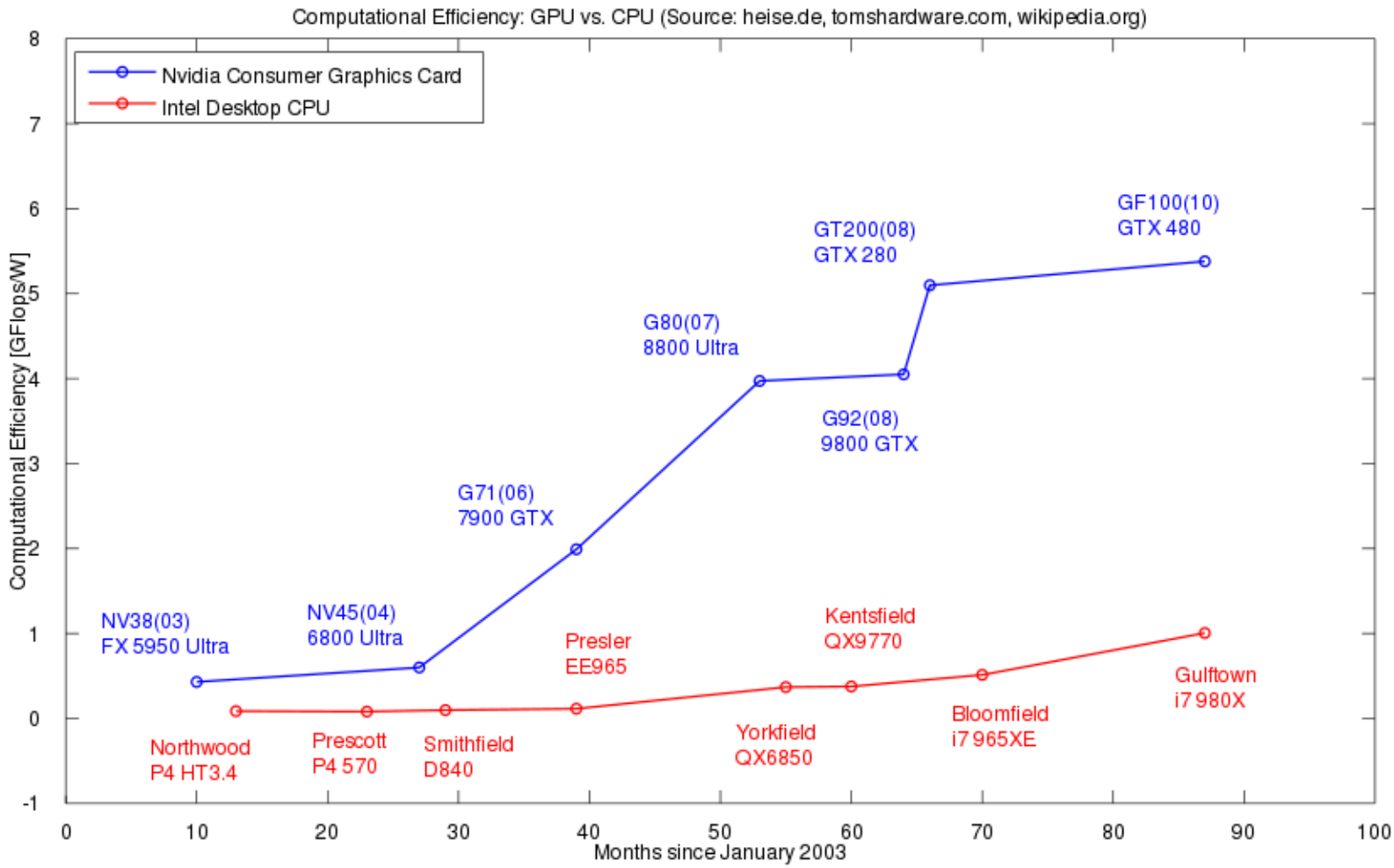
Computational Efficiency: GPU vs. CPU (Source: heise.de, tomshardware.com, wikipedia.org)
Nvidia Consumer Graphics Card
Intel Desktop CPU
Computational Efficiency [GFlops/W]
Months since January 2003
NV38(03)
FX 5950 Ultra
NV45(04)
6800 Ultra
G71(06)
7900 GTX
G80(07)
8800 Ultra
G92(08)
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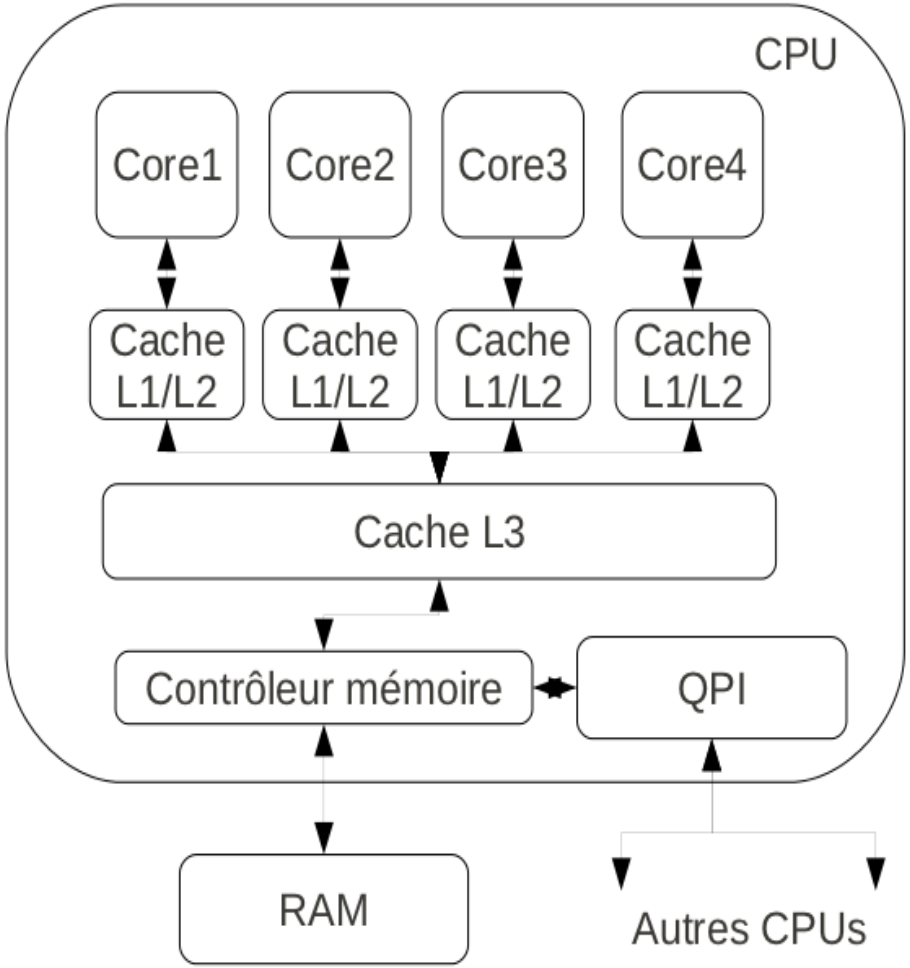
Kentsfield
QX9770
Bloomfield
i7 965XE
Gulftown
i7 980X

CPU versus GPU: deep differences

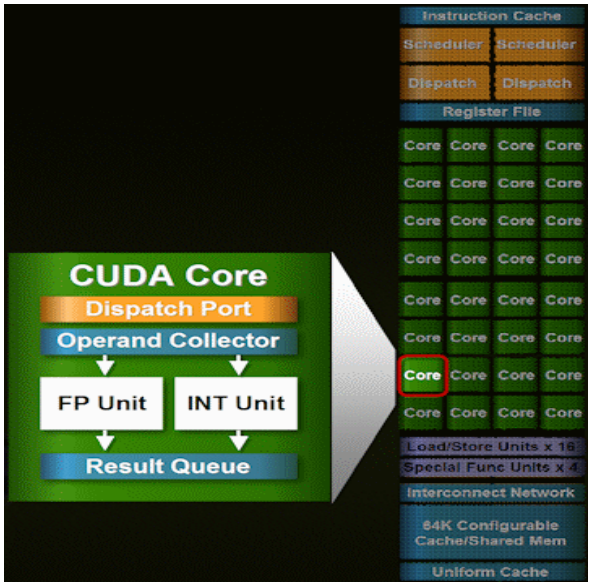
CPU Architecture

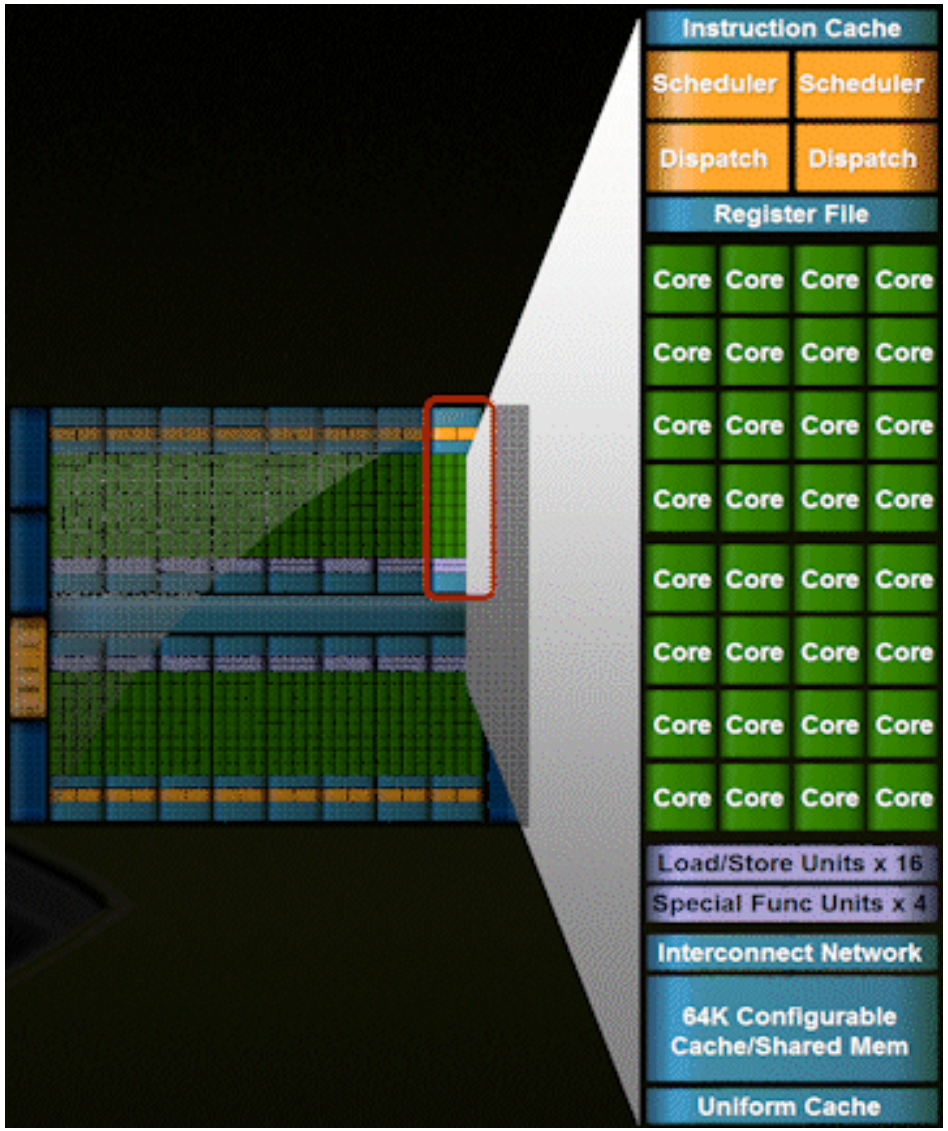
- core i7
  - Real quadri cores
  - Hyper Threading
    - 8 threads simultaneously
  - QPI
    - Point to point interconnection
    - Up to 4 CPU
    - 4 * 4 * 2 = 32 threads simultaneously



GPU Architecture (NVIDIA Card)

- SP (1 scalar)
- Streaming Multiprocessor SM
  - 32 SP
  - 4SFU
  - M-Thread Ctl
  - Shared Memory





We need new programming language... again...

- To exploit all resources of these hardware and facilitate programming
- Several solutions are available:
  - NVIDIA CUDA C
    - provides a low level and a high level API
    - works only on NVIDIA Card
  - OpenCL
    - frameworks for writing programs
    - can be executed across heterogeneous platforms consisting of CPUs, GPUs, and other processors
  - PGI CUDA Fortran
    - wrappers of NVIDIA CUDA C
    - tool chain for programming in Fortran
  - PGI Accelerator
    - implementation by directives (like OpenMP)
    - easy-to-begin

CUDA: an API with new concepts

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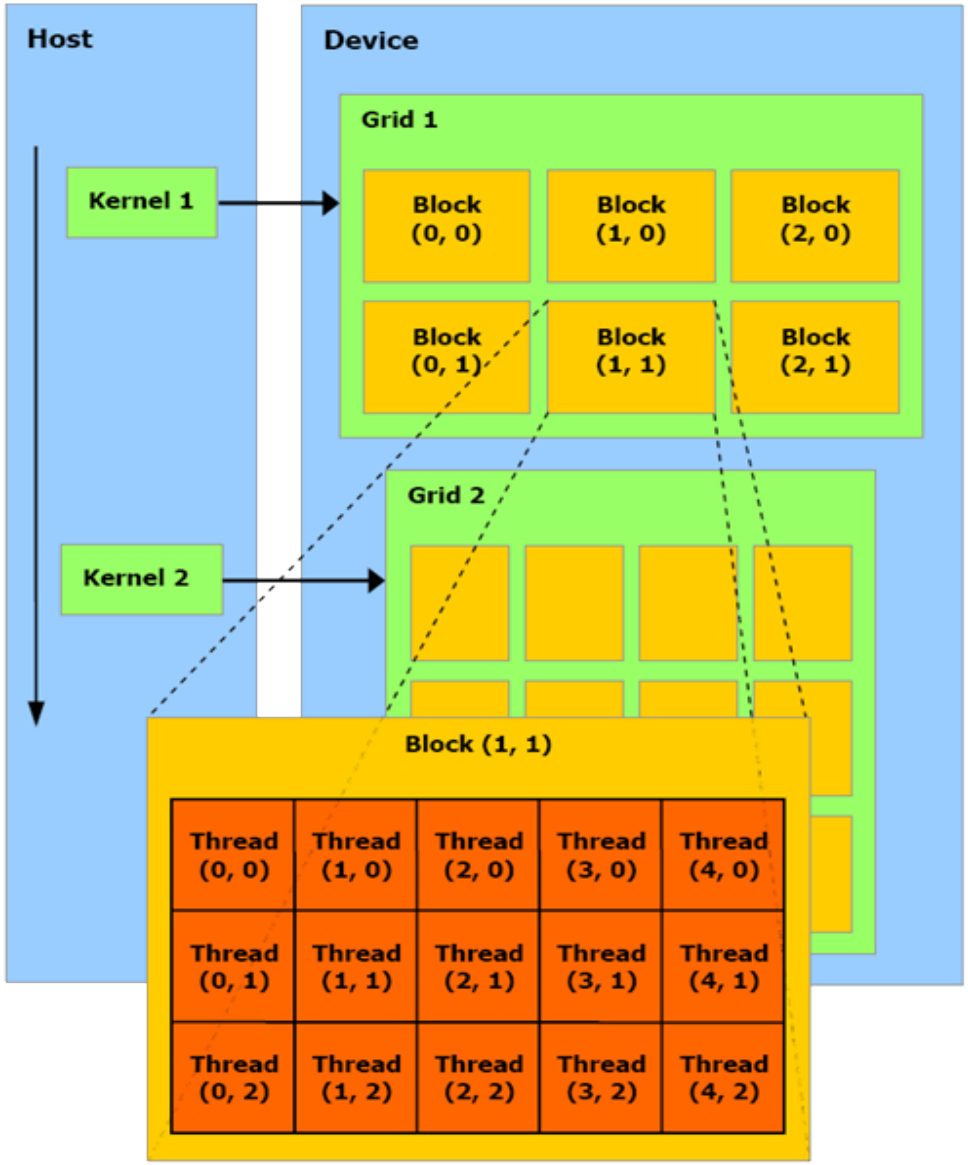
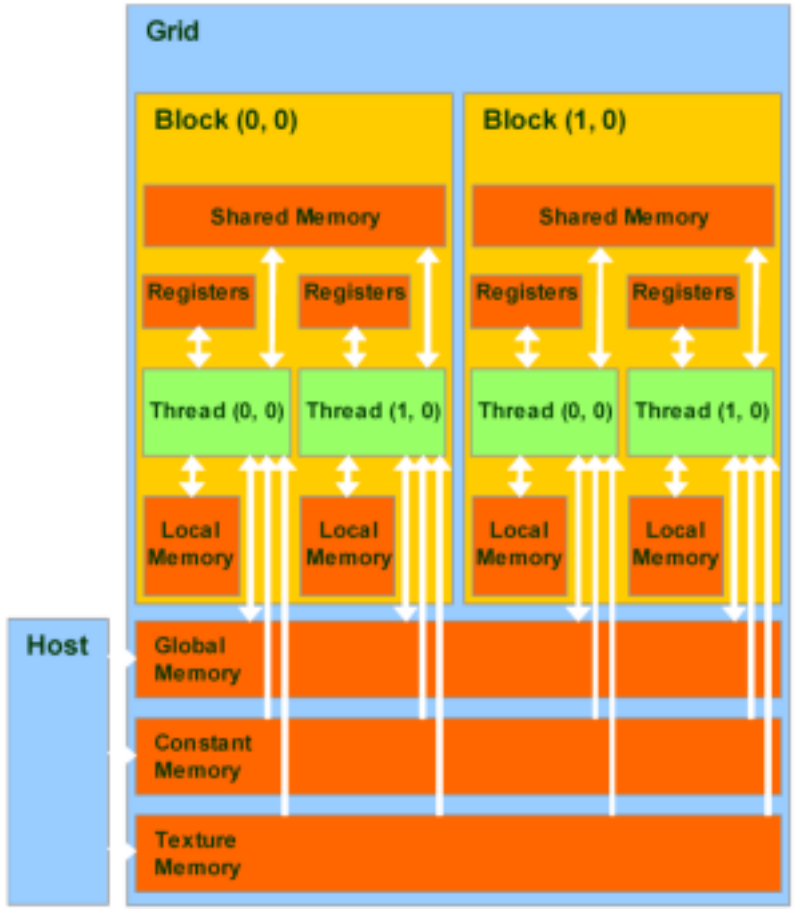
Grid and blocs

- Grid
  - set of blocks
- Blocks
  - set of threads
  - each block are independent
  - each blocks have a specific shared memory
- Threads
  - each thread runs an instance of kernel
  - threads can be synchronized in a block
  - all thread can exchange data thanks to shared memory
- Warp
  - set of n threads (n=32 for C2070)
  - these n threads are run simultaneously
  - a warp is run over 2 cycles



Memory space overview

- Each thread can:
  - R/W per-thread registers
  - R/W per-thread local memory
  - R/W per-block shared memory
  - R/W per-grid global memory
  - Read only per-grid constant memory
  - Read only per-grid texture memory
- The host can R/W global, constant, and texture memories



The useful functions

CUDA C:

- Memory management:
  - cudaMalloc(&Md, size * sizeof * Md);
  - cudaMemcpy(Md, M, size * sizeof * Md);
  - cudaFree(Md);
- Device management:
  - cudaSetDevice (devnum);
  - cudaGetDevice (devnum);
  - cudaGetDeviceProperties (prop, devnum);

CUDA Fortran:

- Memory management:
  - call cudaMalloc(devptr, count)
  - call cudaMemcpy(dst, src, count, kdir)
  - call cudaFree(devptr)
- Device management:
  - call cudaSetDevice(devnum)
  - call cudaGetDevice(devnum)
  - call cudaGetDeviceProperties (prop, devnum)

Extensions and Kernels (1/2)

CUDA C:

- Function qualifiers:
  - __global__ void kernel() { }
  - __device__ void fromdev() {}
  - __host__ void fromhost(){}
- Variable qualifiers:
  - __shared__ float tile[][];
  - __device__ int GlobalVar;
  - __constant__ int Var;

CUDA Fortran:

- Subroutine qualifiers:
  - attributes(global) subroutine my_kernel (...)
  - attributes(device) subroutine my_kernel (...)
  - attributes(host) subroutine my_kernel (...)
- Variable qualifiers:
  - <type>, device :: x
  - <type>, constant :: x
  - <type>, shared :: x
  - <type>, pinned :: x
  - <type>, value :: x

Extensions and Kernels (2/2)

CUDA C:

- Built-in variables and functions valid in device code:
  - dim3 bDim, gDim;
  - gDim(32,32,0);
  - bDim(32,32,32);
  - kernel<<<gDim, bDim>>>(...);
- Execution configurations:
  - gridDim.{x, y, z}
  - blockDim.{x,y,z}
  - blockIdx.{x,y,z}
  - threadIdx.{x, y, z}
  - __syncthreads();

CUDA Fortran:

- Built-in variables and functions valid in device code:
  - type(dim3) :: dimGrid, dimBlock
  - dimGrid = dim3(32, 32, 0)
  - dimBlock = dim3(32, 32, 32)
  - call my_kernel <<<dimGrid, dimBlock>>> (...)
- Execution configurations:
  - gridDim%{x, y, z}
  - blockDim%{x, y, z}
  - blockIdx%{x, y, z}
  - threadIdx%{x, y, z}
  - call syncthreads()

Compilation

CUDA C:

- Compiler + CUDA Toolkit
- file: .cu
  - compiler: nvcc
  - link: cudart
- nvcc *.cu -lcudart -o prog

PGI CUDA Fortran:

- Only PGI Compiler
- file: .cuf .CUF
  - compiler:pgfortran
  - link: cuda
- pgfortran -Mcuda *.cuf -o prog

Differences between CUDA C and Fortran

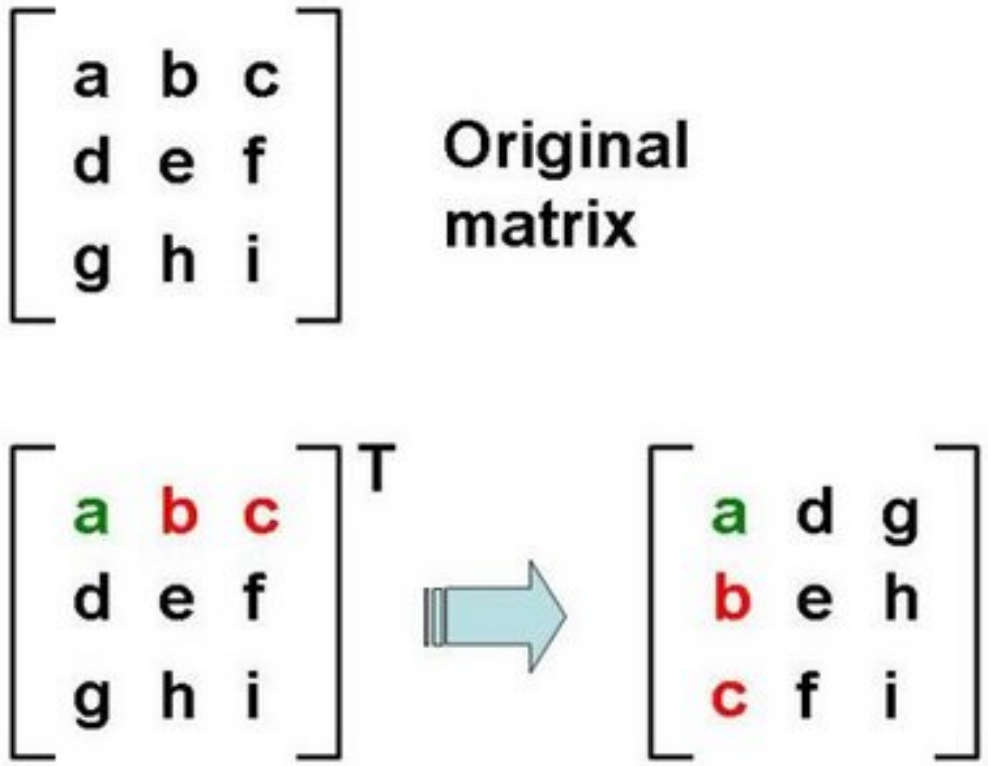
- CUDA C supports
  - texture memory
  - Runtime API
  - Drivers API
- Interoperability with
  - OpenGL
  - Direct3D
- Indexing
  - arrays 0-based
  - threadIdx and blockIdx 0-based

- CUDA Fortran don't support
  - texture memory
  - Runtime API
  - Drivers API
- No interoperability with
  - OpenGL
  - Direct3D
- Indexing
  - arrays 1-based
  - threadIdx and blockIdx 1-based

Why make it simple when it can be complicated?

Example 1: Transpose matrix

- Example of data shaking-up
  - common in algorithms for optimizations
  - data moving only, no data treatments
- Example similar to copy
  - give a reference
  - simple to implement
- We need an indicator : bandwidth
  - here, bandwidth = [memory size of the matrix] / [time]
  - warning: effective bandwidth = [2 * memory size of the matrix] / [time]



Transpose matrix: Host code (1/2)

Source Code in CUDA C:

```
int main (int args, char* argv[])
{

const int HEIGHT = 1024;
const int WIDTH   = 1024;

const int SIZE=WIDTH*HEIGHT*sizeof(float);

float* M   = (float*)malloc(SIZE);
float* Md = NULL;
float* Id   = NULL;
cudaMalloc((void**)&Md, SIZE);
cudaMalloc((void**)&Id, SIZE);

dim3 bDim(16, 16);
dim3 gDim(WIDTH / bDim.x, HEIGHT / bDim.
y);

transpose<<<gDim, bDim>>>(Md, Bd, WIDTH);

cudaFree(Md);
cudaFree(Id);

free(M);

return 0;

}
```

Transpose matrix: Host code (2/2)

Source Code in CUDA Fortran:

```
program cuda_transpose
    use cudafor
    implicit none

    type(dim3) :: dimGrid, dimBlock
    real, allocatable, device :: an_d(:,:),at_d(:,:)
    real, allocatable :: an(:,:), at(:,:)
    real :: alpha, beta
    integer :: m, l

    m = 1024 ; l = 1024
    allocate (an(m,l), at(l,m))
    allocate (an_d(m,l), at_d(l,m))

    a = 1.0 ; b = 2.0 ; c = 3.0
    alpha = 1.0 ; beta  = 0.0

    dimGrid  = dim3(m/32, l/32, 1)
    dimBlock = dim3(32, 8, 1)

    an_d = an
    call matrix_transpose_direct<<< dimGrid,
dimBlock >>>(an_d, at_d, m, l)
    at = at_d

    deallocate (an,at)
    deallocate (an_d,at_d)
end program cuda_transpose
```

Simple-minded implementation (1/2)

Idea:

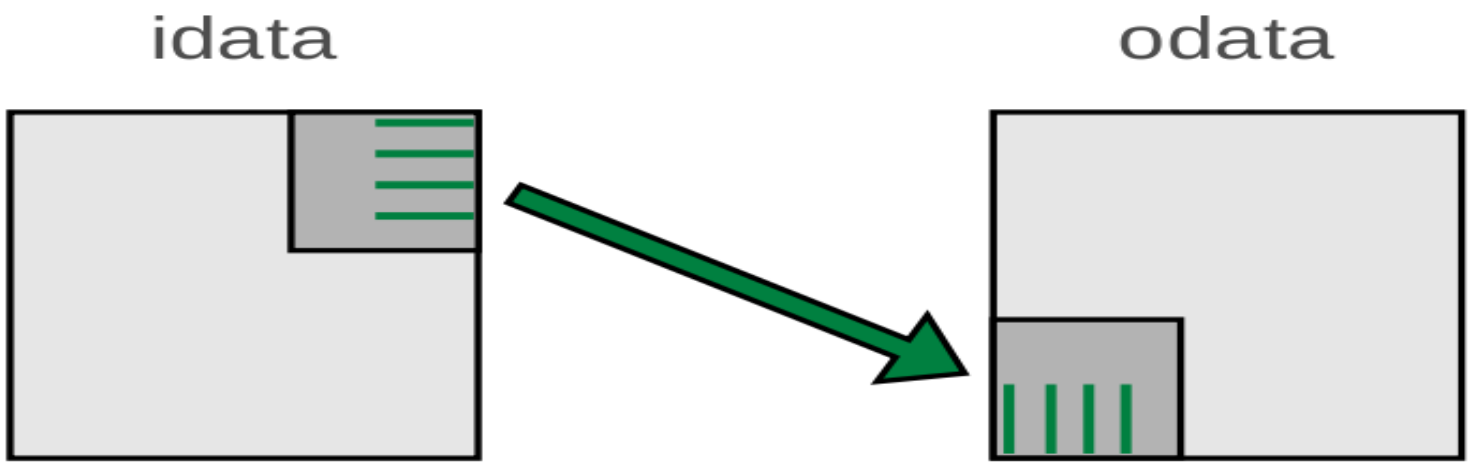
- compute four values by thread
- direct transfers from/to global memory
- kernel very similar to CPU code

Why?

- easy-to-write
- very simple (maybe too simple?)

Parameter of the kernel:

- dimGrid = (m/32, l/32, 1)
- dimBlock = (32, 8, 1)



Simple-minded implementation (2/2)

Source Code in CUDA C:

```
 __global__ void transpose
(float* in, float* out, uint width)

{

  uint tx = blockIdx.x * blockDim.x + threadIdx.x;
  uint ty = blockIdx.y * blockDim.y + threadIdx.y;

      out[tx * width + ty] = in[ty * width + tx];

}
```

Source Code in CUDA Fortran:

```
attributes(global) subroutine matrix_transpose
(an, at, m, n)
   implicit none
   real, intent(in) :: an(m,n)
   real, intent(out) :: at(m,n)
   integer, value :: m, n
   integer :: i, ix, iy

   ix = (blockIdx%x-1) * blockDim%x +
threadIdx%x
   iy = (blockIdx%y-1) * blockDim%y +
threadIdx%y

   do i = 0, blockDim%x-1, 8
      at(iy+i,ix) = an(ix,iy+i)
   enddo

end subroutine matrix_transpose
```

Use shared memory, it exists for a reason... (1/2)

Idea:

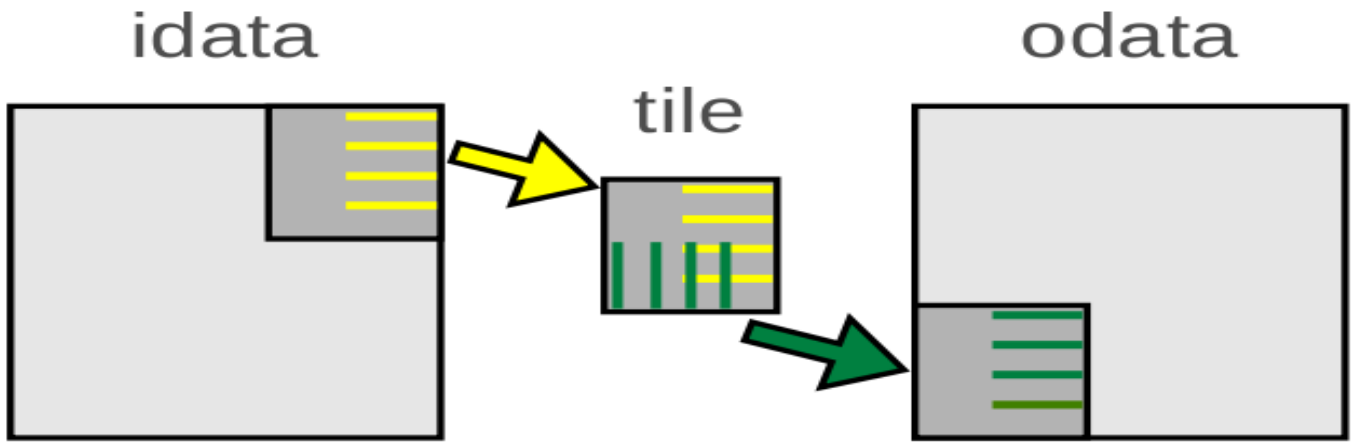
- Compute four values of C by thread again
- each thread wrtie in shared memory
- synchronize all threads
- each thread read in shared memory

Why?

- shared memory have lower latency
- shared memory have higher bandwidth
- more control on access memory

Parameter of the kernel:

- dimGrid = (m/32, l/32, 1)
- dimBlock = (32, 8, 1)



Use shared memory, it exists for a reason... (2/2)

Source Code in CUDA C:

```
 __global__
void transpose
(float* in, float* out, uint width)
{
__shared__ float tile[32][32];

__shared__ int i;
__shared__ int block;
uint tx = blockIdx.x * blockDim.x + threadIdx.x;
uint ty = blockIdx.y * blockDim.y + threadIdx.y;

block = width / 32;

for(i = 0; i < 32; i+= block)
tile[threadIdx.y + i][threadIdx.x] = in[ty * width + tx];

for(i = 0; i < 32; i+= block)
out[tx * width + ty + i * width] = tile[threadIdx.x]
[threadIdx.y + i];

}
```

Source Code in CUDA Fortran:

```
attributes(global) subroutine matrix_transpose(an, at, m, n)
  implicit none
  real, intent(in) :: an(m,n)
  real, intent(out) :: at(m,n)
  real, shared :: tile(32,32)
  integer, value :: m, n
  integer :: i, ix, iy, tx, ty

  tx  = threadIdx%x
  ty  = threadIdx%y
  ix = (blockIdx%x-1) * blockDim%x + tx
  iy = (blockIdx%y-1) * blockDim%x + ty
  do i = 0, blockDim%x, 8
       tile(tx,ty+i) = an(ix,iy+i)
  enddo
  call syncthreads()

  ix = (blockIdx%y-1) * blockDim%x + tx
  iy = (blockIdx%x-1) * blockDim%x + ty
  do i = 0, blockDim%x-1, 8
    at(ix,iy+i) = tile(ty+i,tx)
  enddo
end subroutine matrix_transpose
```

We can do more complicated... Partition camping (1/2)

Idea:

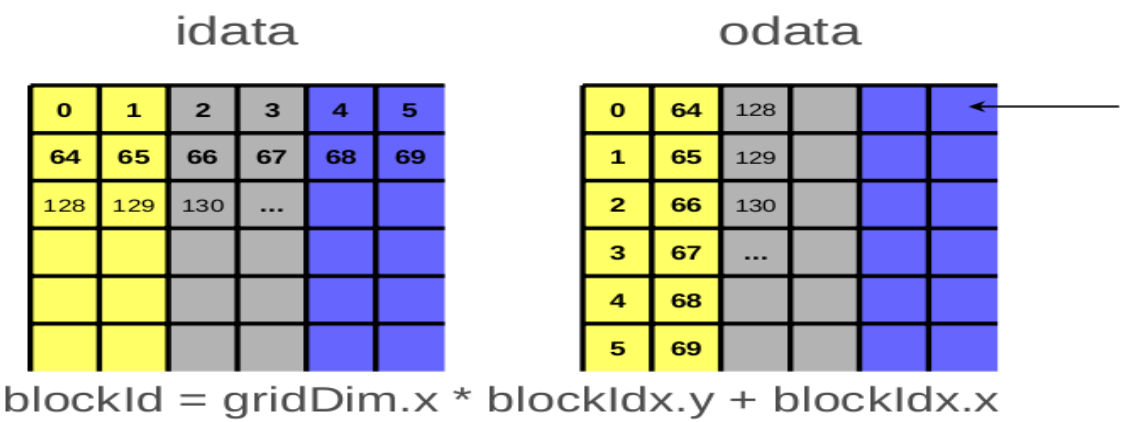
- Compute four values of C by thread again
- reordering blockIdx to force diagonalized numbering
- used of shared memroy

Why?

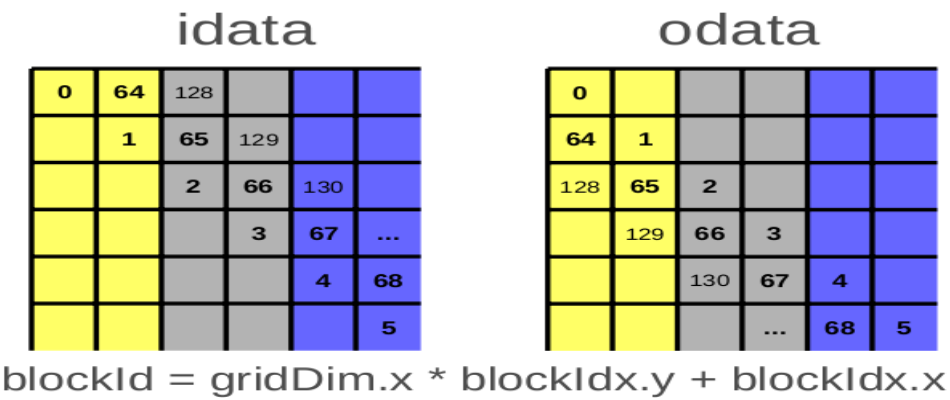
- avoid partition camping ie avoid concurrency access memory
- more control on access memory

Parameter of the kernel:

- dimGrid = (m/32, l/32, 1)
- dimBlock = (32, 8, 1)



tiles in matrices
colors = partitions

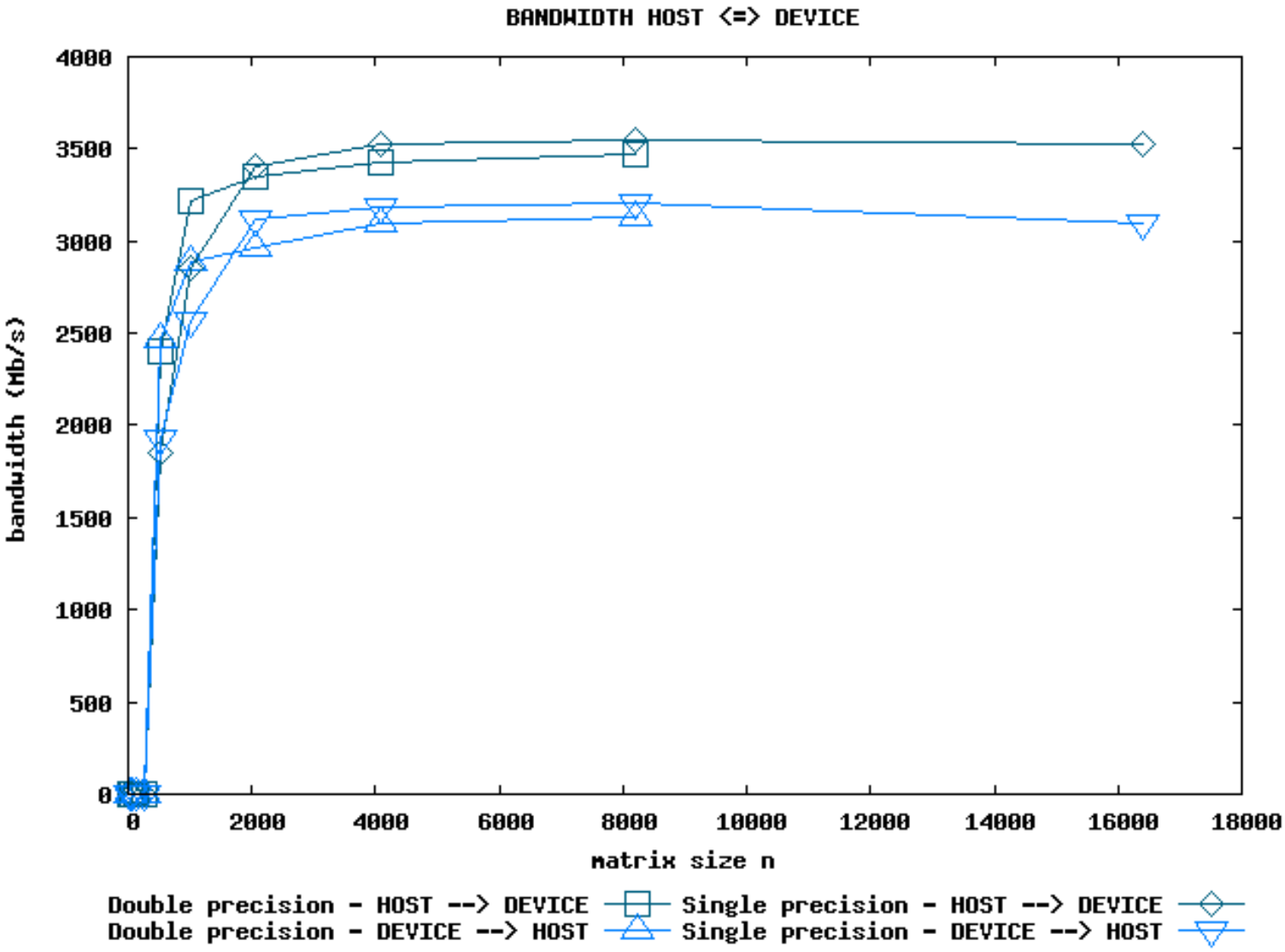


We can do more complicated... Partition camping (2/2)

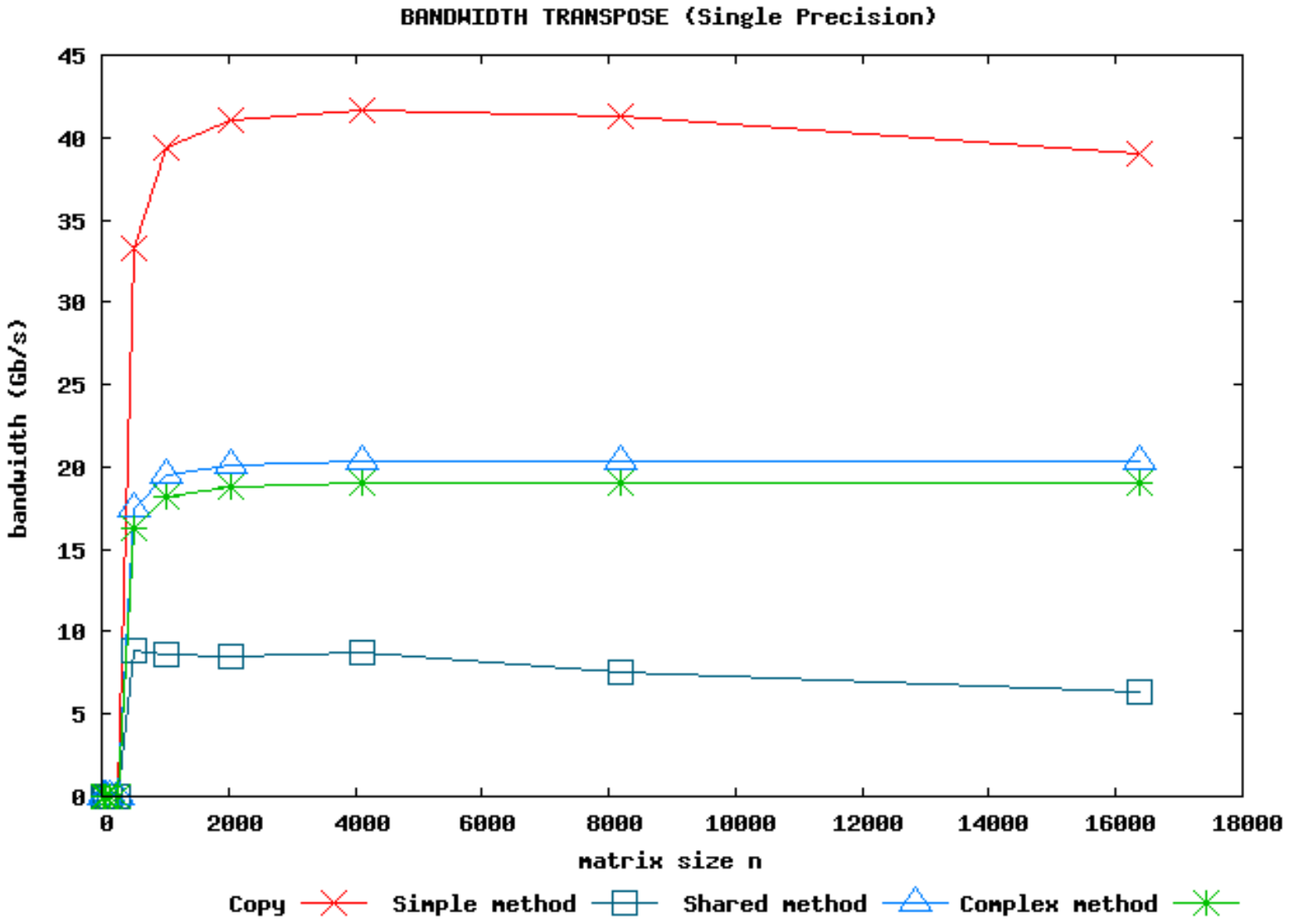
Source Code in CUDA Fortran:

```
attributes(global) subroutine matrix_transpose(an, at,
m, n)
  implicit none
  real, intent(in) :: an(m,n)
  real, intent(out) :: at(m,n)
  real, shared :: tile(32,32)
  integer, shared :: ibx, iby
  integer, value :: m, n
  integer :: i, ix, iy, tx, ty, ibid

  tx  = threadIdx%x
  ty  = threadIdx%y
  if (m==n) then
    iby = blockIdx%x-1
    ibx = mod(blockIdx%x+blockIdx%y-2, gridDim%x)
  else
    ibid = gridDim%x*(blockIdx%y-1) + blockIdx%x -
1
    iby = mod(ibid, gridDim%y)
    ibx = mod(ibid/gridDim%y+iy, gridDim%x)
  endif
  ibx = ibx * blockIdx%x
  iby = iby * blockIdx%x

  ix = ibx + tx
  iy = iby + ty
  do i = 0, blockIdx%x-1, 8
    tile(tx,ty+i) = an(ix,iy+i)
  enddo
  call syncthreads()

  ix = iby + tx
  iy = ibx + ty
  do i = 0, blockIdx%x-1,8
    at(ix,iy+i) = tile(ty+i,tx)
  enddo

end subroutine matrix_transpose
```

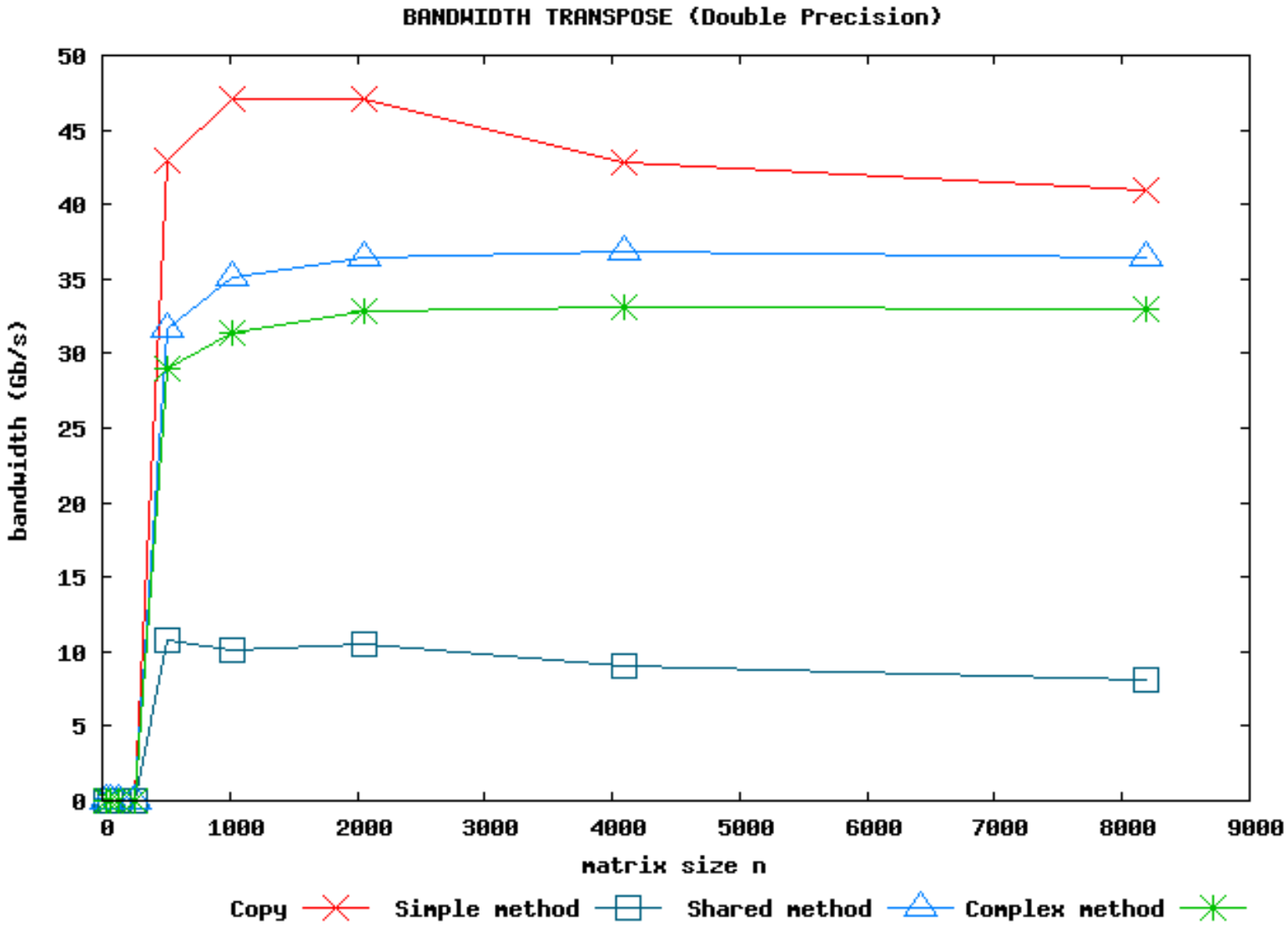
Which performance in the end?



Which performance in the end?

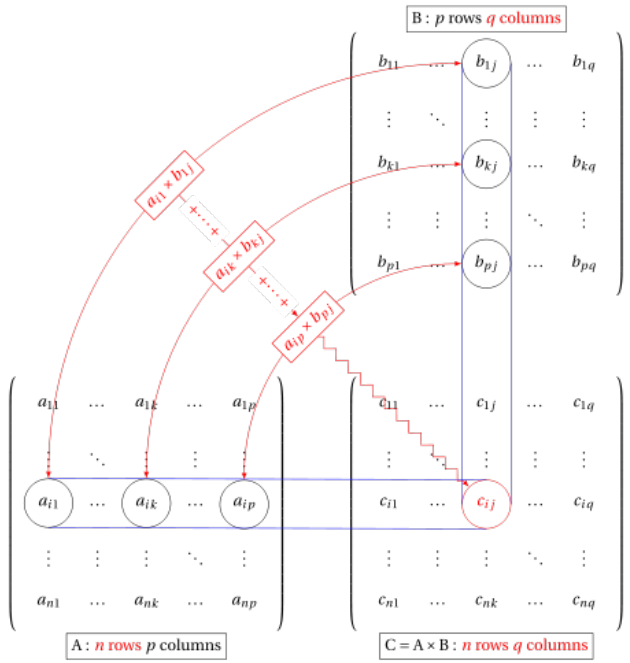


Which performance in the end?

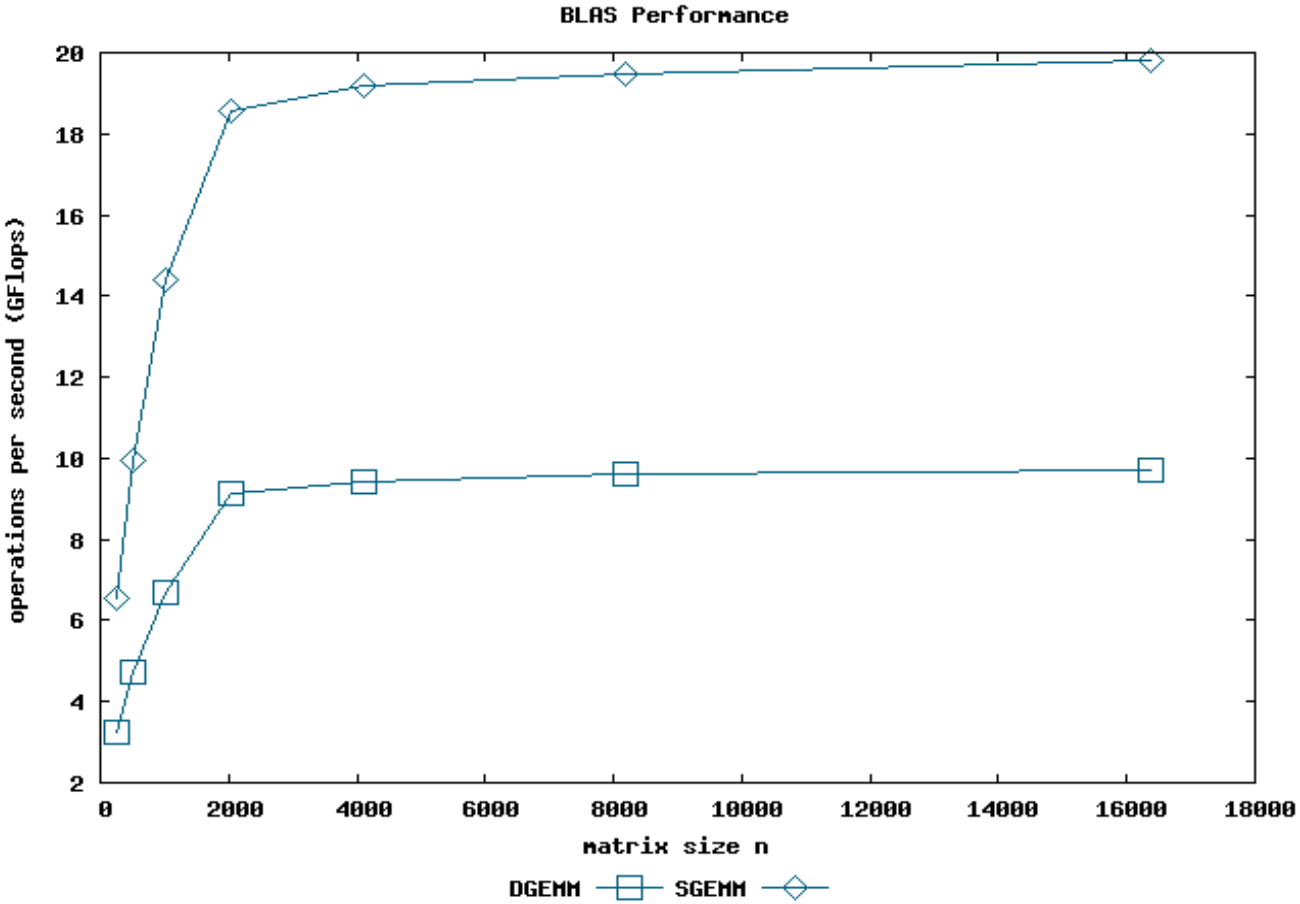


Example 2: Matrix multiplication

- Common algorithm:
  - "school example"
  - use for benchmarking
- We need an indicator : Flops or Floating Point Operations Per Second:
  - Flops = [number of operations of the algorithm] / [time]
  - here: number of operations of the algorithm= n * q * (2p+2)
  - if square matrices : complexity in $O(n^3)$



Performance on CPU



- Intel ComposerXE 12.0 + Intel MKL 10.3
- <t>GEMM in multithread version
- Test machine: one node "mirage" on PlaFRIM
- Benchmkark over 12 thread

Simple-minded implementation (1/2)

Idea:

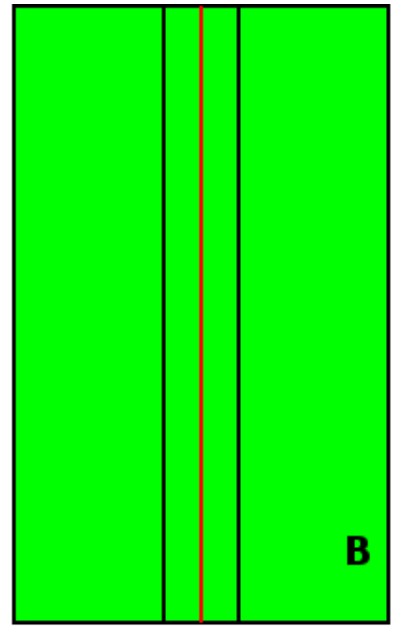
- compute one value of C by thread
- run on one row of A and one column of B by thread
- direct access from/to global memory
- kernel very similar to CPU code

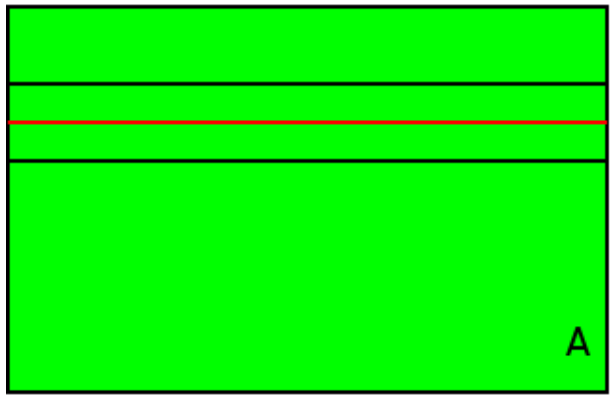
Why?

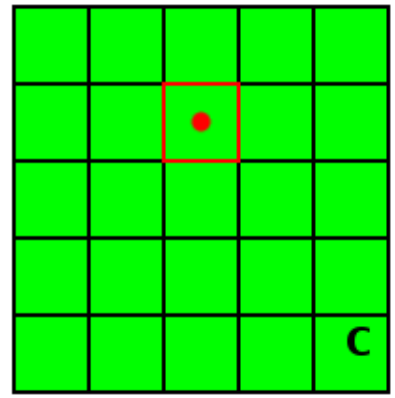
- easy-to-write
- very simple (maybe too simple?)

Parameter of the kernel:

- dimGrid = (m/32, n/32, 1)
- dimBlock = (32, 32, 1)







Simple-minded implementation (2/2)

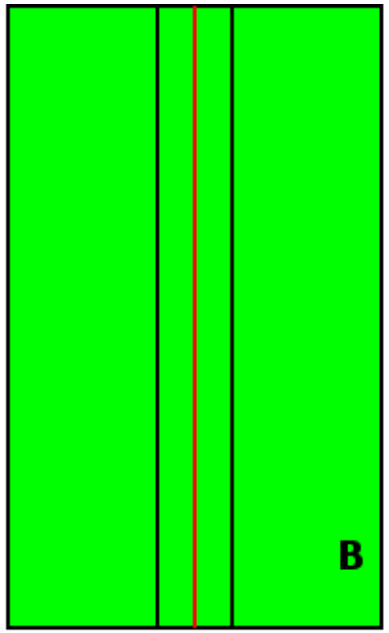
Source Code in CUDA C:

```
 __global__
void MatrixMulKernel
(float * Md, float * Nd, float * Pd, int Width)
{

  uint tx = blockIdx.x * blockDim.x + threadIdx.x;
  uint ty = blockIdx.y * blockDim.y + threadIdx.y;

   float Pvaleur = 0;
   float MdElement , NdElement;
   for (i = 0; i < Width; i++)
    {
       MdElement = Md[threadIdx.y * Width + i];
       NdElement = Nd[i  * Width + threadIdx.x];
       Pvaleur+=MdElement*NdElement;
    }

    Pd[ty * Width + tx] = Pvaleur;

}
```

Source Code in CUDA Fortran:

```
attributes(global) subroutine matrix_mul(a, b, c, m, l, n)
  implicit none
  real(fp_kind), intent(in) :: a(l,m), b(l,n)
  real(fp_kind), intent(out) :: c(m,n)
  integer, value :: m, l, n
  real(fp_kind) :: cij
  integer :: k, ix, iy

  ix = (blockIdx%x-1) * dimBlock%x + threadIdx%x
  iy = (blockIdx%y-1) * dimBlock%y + threadIdx%y

  cij = 0.0
  do k=1,l
    cij = cij + a(k,ix)*b(k,iy)
  enddo

  c(ix,iy) = cij
end subroutine matrix_mul
```

Use shared memory for matrix A (1/2)

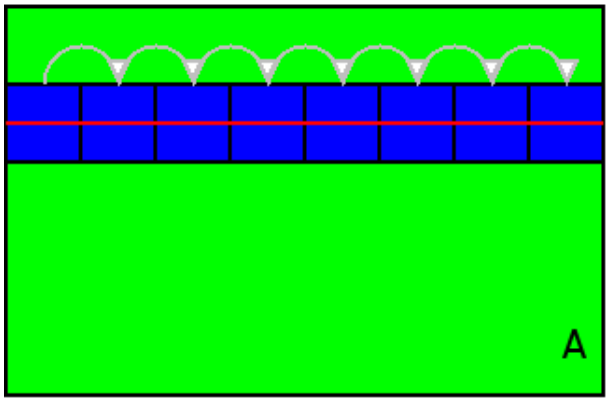


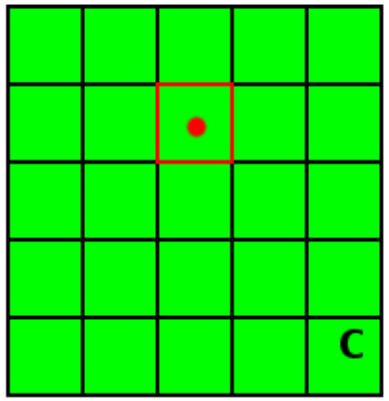
Idea:

- compute one value of C by thread
- run on one row of A and one column of B by thread
- store parts of rows of A in shared memory
- have to iterate to put all the row of A in shared memory
- direct access from global memory for B

Why?

- shared memory have lower latency
- shared memory have higher bandwidth
- more control on access memory





Parameter of the kernel:

- dimGrid = (m/32, n/32, 1)
- dimBlock = (32, 32, 1)

Use shared memory for matrix A (2/2)

Source Code in CUDA C:

```
 __global__
void MatrixMulKernel
(float * Md, float * Nd, float * Pd, int Width)
{
   int i;
   __shared__ float aTile[32][32];

  uint tx = blockIdx.x * blockDim.x + threadIdx.x;
  uint ty = blockIdx.y * blockDim.y + threadIdx.y;

   float Pvaleur = 0;
   float MdElement , NdElement;
   for (i = 0; i < Width; i++)
    {
        NdElement = Nd[i  * Width + threadIdx.x];
       Pvaleur+=aTile[tx][ty]*NdElement;
    }

  Pd[ty * Width + tx] = Pvaleur;
}
```

Source Code in CUDA Fortran:

```
attributes(global) subroutine matrix_mul(a, b, c, m, l, n)
  implicit none
  real, intent(in) :: a(l,m), b(l,n)
  real, intent(out) :: c(m,n)
  integer, value :: m, l, n
  real, shared :: a_shared(32, 32)
  real :: cij
  integer :: i, j, ix, iy, tx, ty

  tx  = threadIdx%x ; ty  = threadIdx%y
  ix = (blockIdx%x-1) * dimGrid%x + tx
  iy = (blockIdx%y-1) * dimGrid%y + ty

  cij = 0.0
  do i = 1, l, 32
    a_shared(tx,ty) = a(i+ty-1, ix)
    call syncthreads()
    do j = 1, 32
      cij = cij + a_shared(tx,j)*b(i+j-1, iy)
    enddo
    call syncthreads()
  enddo
  c(ix,iy) = cij
end subroutine matrix_mul
```

Use shared memory for matrix A and B (1/2)

<u>Idea:</u>

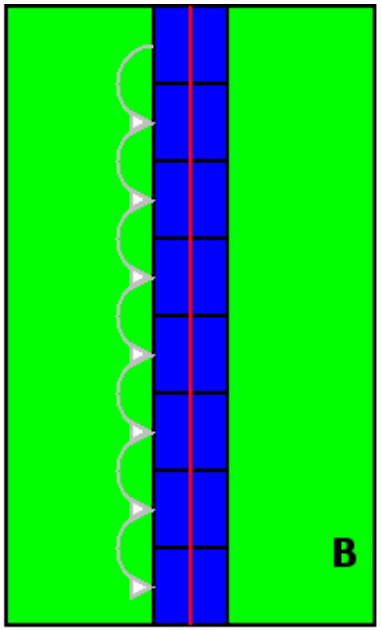
- compute one value of C by thread
- run on one row of A and one column of B by thread
- store parts of rows of A and B in shared memory
- have to iterate to put all the row of A and B in shared memory
- increase number of iterations

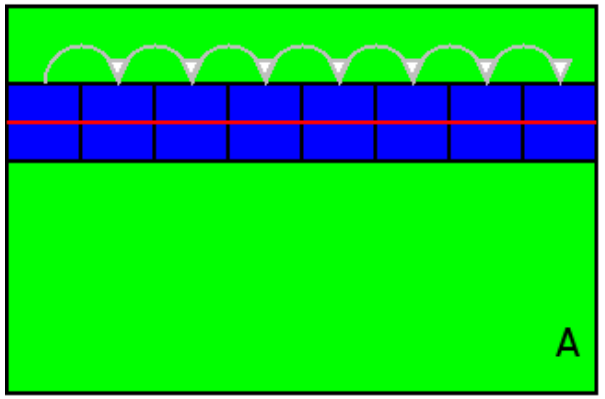
<u>Why?</u>

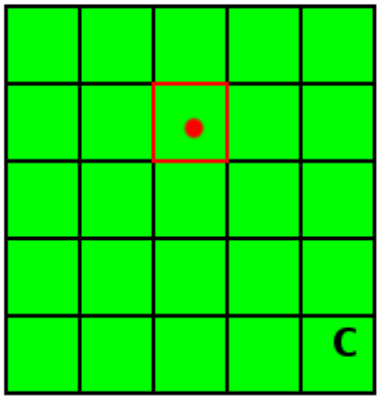
- shared memory have lower latency
- shared memory have higher bandwidth
- more control on access memory

<u>Parameter of the kernel:</u>

- dimGrid = (m/16, n/16, 1)
- dimBlock = (16, 16, 1)





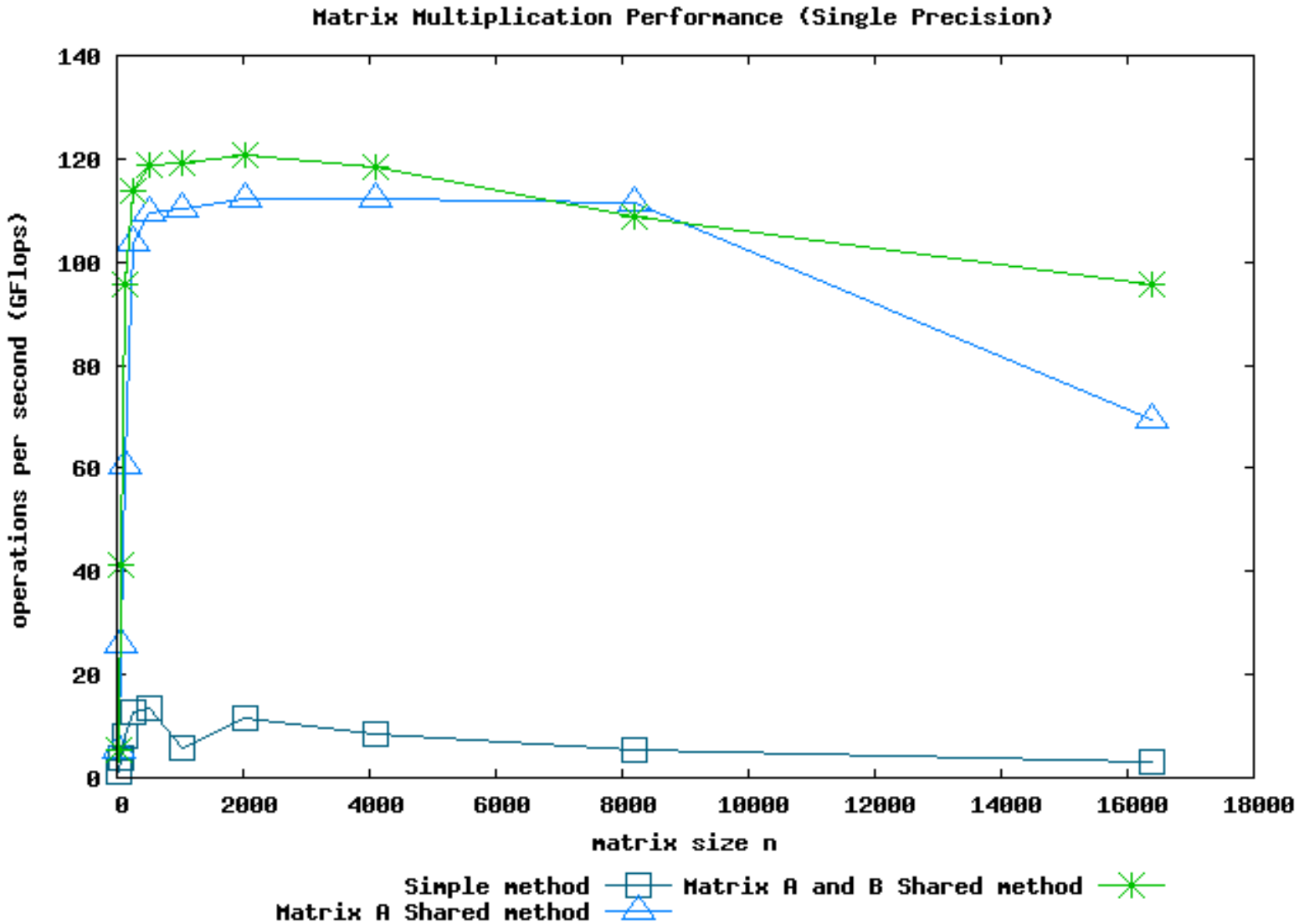


Use shared memory for matrix A and B (2/2)

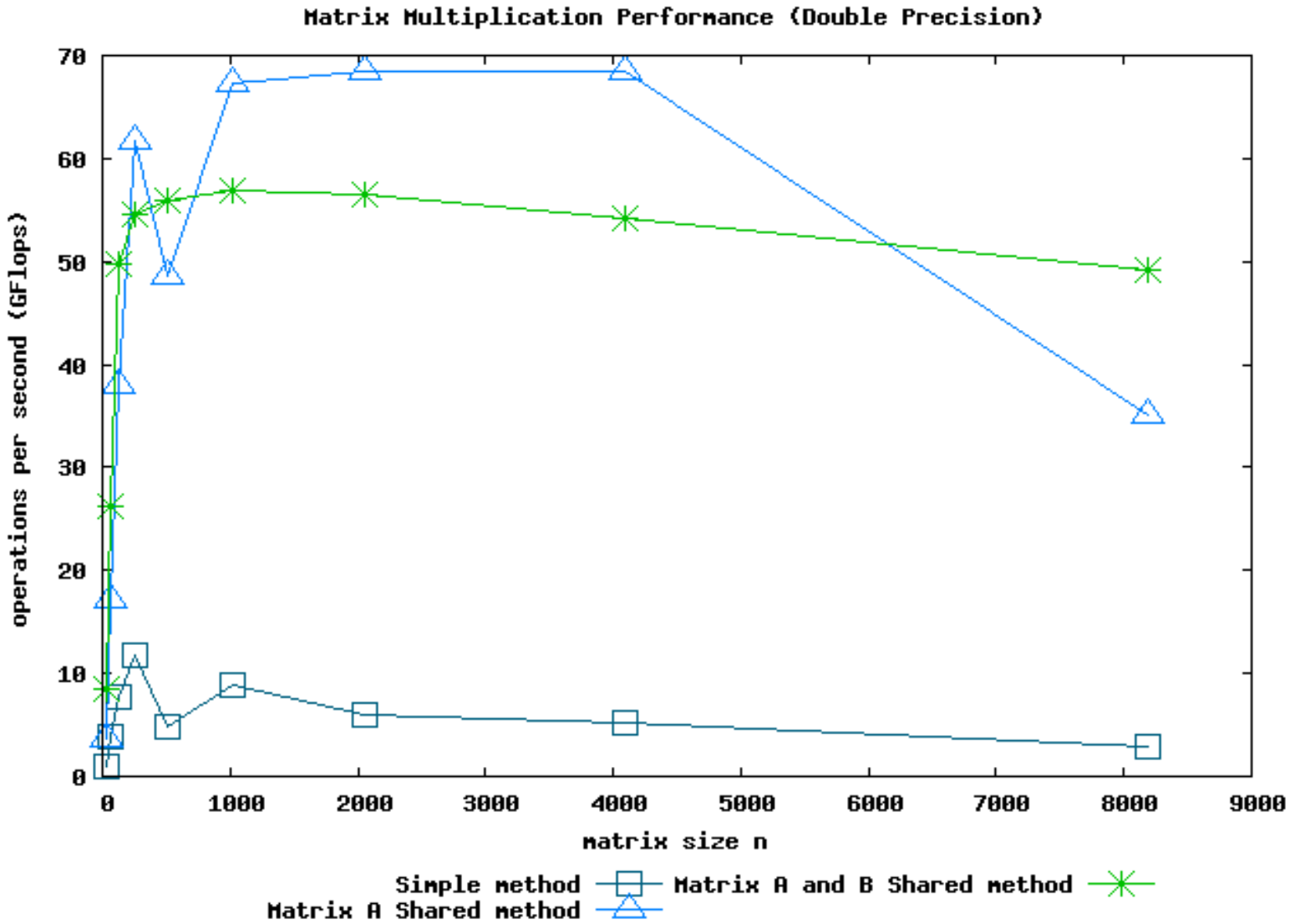
Source Code in CUDA Fortran:

```
attributes(global) subroutine matrix_mul(a, b, c, m, l,
n)
  implicit none
  real(fp_kind), intent(in) :: a(l,m), b(l,n)
  real(fp_kind), intent(out) :: c(m,n)
  integer, value :: m, l, n
  real(fp_kind), shared :: a_shared(16, 16)
  real(fp_kind), shared :: b_shared(16, 16)
  real(fp_kind) :: cij
  integer :: i, j, ix, iy, tx, ty

  tx  = threadIdx%x
  ty  = threadIdx%y
  ix = (blockIdx%x-1) * blockDim%x + tx
  iy = (blockIdx%y-1) * blockDim%y + ty

  cij = 0.0

  do i = 1, l, 32

    a_shared(tx,ty) = a(i+ty-1, ix)
    b_shared(tx,ty) = b(i+tx-1, iy)
    call syncthreads()

    do j = 1, 32
      cij = cij + a_shared(tx,j)*b_shared(j,ty)
    enddo
    call syncthreads()

  enddo
  c(ix,iy) = cij

end subroutine matrix_mul
```

Which performance in the end?



Which performance in the end?



Help me! Where are the libraries?

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DE RECHERCHE
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BORDEAUX - SUD-OUEST

Libraries for CUDA?

- CUBLAS
  - set of basic linear algebra routines
  - implementation of BLAS on top of CUDA Runtime
- CUFFT
  - used for data signal processing and solving partial differential equations
  - simple interface for FFT computation on GPU
- NPP
  - used for imaging and video processing
  - like implementation of IPP (Intel) on GPU
- CUSP
  - library for sparse linear algebra and graph computations
  - opensource project on Google Code
- CULA
  - library for solving systems of simultaneous linear equations
  - based-on LAPACK
  - EM Photonics in partnership with NVIDIA

Do not you see BLAS right there?

- (CU)BLAS is an organized library for basic linear algebra in 3 levels:
  - BLAS-1: operations between vectors
  - BLAS-2: operations between a matrix and a vector
  - BALS-3 : operations between matrices
- Our interests : <t>GEMM
  - function performs the matrix-matrix multiplication:

$$C = \alpha op(A) op(B) + \beta C$$

where α and β are scalars,
A, B, C are matrices,
and op() is (conjugate) transpose or not

CUBLAS help to program quickly (1/5)

Source Code in CUDA C:

```
 int main(int argc, char * argv[])
{
int i;
int Width;
int iteration;

double *M;
double *N;
double *P;

void **Md;
void **Nd;
void **Pd;

M = (double*) malloc (size * sizeof(double));
N = (double*) malloc (size * sizeof(double));
P = (double*) malloc (size * sizeof(double));

cublasInit();
cublasAlloc( size , sizeof(double) , (void**)&Md);
cublasSetMatrix(Width,Width,sizeof(double),M,Width,Md,
Width);
cublasAlloc( size , sizeof(double) , (void**)&Nd);
cublasSetMatrix(Width,Width,sizeof(double),N,Width,Nd,
Width);

cublasAlloc( size , sizeof(double) ,(void**)&Pd);

cublasDgemm ('N','N',Width,Width,Width,(double) 1.0,(const
double *)Md,Width,(const double *)Nd,Width,(double) 0.0,
(double *)Pd,Width);

cublasGetMatrix(Width,Width,sizeof(double),Pd,Width,P,
Width);

cublasFree(Md);
cublasFree(Nd);
cublasFree(Pd);

free(M);
free(N);
free(P);

}
```

CUBLAS help to program quickly (2/5)

Options in CUDA Fortran:

- ISO_C_BINDING:
  - binding NVIDIA CUDA C functions to define subroutine
  - using PGI extensions for memory management
- NON Thunking method:
  - using NVIDIA interface with manual memory management
  - using cublasAlloc / cublasFree
  - using cublasSetMatrix / cublasGetMatrix
  - using cublasSGEMM / cublasDGEMM
- Thunking method:
  - using NVIDIA interface with automaticl memory management
  - not need to alloc GPU memory
  - using cublasSGEMM / cublasDGEMM only

CUBLAS help to program quickly (3/5)

ISO C Binding method:

```
interface cuda_gemm
subroutine cuda_sgemm(cta, ctb, m, n, k,alpha,
A, lda, B, ldb, beta, c, ldc) bind(C,
name='cublasSgemm')
   use iso_c_binding
   character(1,c_char),value :: cta, ctb
   integer(c_int),value :: m,n,k,lda,ldb,ldc
   real(c_float),value :: alpha,beta
   real(c_float), device, dimension(lda,*) :: A
   real(c_float), device, dimension(ldb,*) :: B
   real(c_float), device, dimension(ldc,*) :: C
end subroutine cuda_sgemm
end interface cuda_gemm

program cublas_iso_c_binding
    use cudafor
    implicit none
    real, allocatable :: a(:,:), b(:,:), c(:,:)
    real, allocatable, device :: a_d(:,:), b_d(:,:), c_d(:,:)
    real(fp_kind) :: alpha, beta
    integer :: m, l, n
    integer :: i, j, k

    m = 1024 ; l = 1024 ; n = 1024
    allocate (a(m,l), b(l,n), c(m,n))

    a = 1.0 ; b = 2.0 ; c = 3.0
    alpha = 1.0 ; beta  = 0.0

    allocate (a_d(m,l), b_d(l,n), c_d(m,n))
    a_d = a ; b_d = b

    call cuda_gemm ('N','N',m,n,l,alpha,a_d,m,b_d,l,
beta,c_d,m)
    c = c_d

    deallocate (a,b,c)
    deallocate (a_d, b_d, c_d)
end program cublas_iso_c_binding
```

CUBLAS help to program quickly (4/5)

Non thunking method:

```
program cublas_non_thunking
   implicit none
   real, allocatable :: a(:,:), b(:,:), c(:,:)
   type(c_ptr) :: a_d, b_d, c_d
   real :: alpha, beta
   integer :: m, l, n, fp_kind=4

   m = 1024 ; l = 1024 ; n = 1024
   allocate (a(m,l), b(l,n), c(m,n))

   a = 1.0 ; b = 2.0 ; c = 3.0
   alpha = 1.0 ; beta  = 0.0

   call cublas_Init()
   call cublas_Alloc(m*l, fp_kind, a_d)
   call cublas_Alloc(l*n, fp_kind, b_d)
   call cublas_Alloc(m*n, fp_kind, c_d)
   call cublas_Set_Matrix(m, l, fp_kind, a, l, a_d, l)
   call cublas_Set_Matrix(l, n, fp_kind, b, n, b_d, n)

   call cublas_SGEMM('n', 'n', m, n, l, alpha, a_d, l,
b_d, n, beta, c_d, n)
   call cublas_Get_Matrix(m, n, fp_kind, c_d, n, c, n)

   deallocate (a,b,c)
   call cublas_Free(a_d)
   call cublas_Free(b_d)
   call cublas_Free(c_d)
   call cublas_Shutdown()

end program cublas_non_thunking
```

CUBLAS help to program quickly (5/5)

Non thunking method:

```
program cublas_thunking
    implicit none
    real, allocatable :: a(:,:), b(:,:), c(:,:)
    real :: alpha, beta
    integer :: m, l, n

    m = 1024 ; l = 1024 ; n = 1024
    allocate (a(m,l), b(l,n), c(m,n))

    a = 1.0 ; b = 2.0 ; c = 3.0
    alpha = 1.0 ; beta  = 0.0

    call cublas_SGEMM('n', 'n', m, n, l, alpha, a, l, b, n, beta, c, n)

    deallocate (a,b,c)
end program cublas_thunking
```

Compilation

CUDA C with CuBLAS:

```
module load compiler/gcc gpu/cuda/3.2.16
nvcc *.cu -lcudart -o prog
```

ISO C Binding:

```
module load compiler/pgi gpu/cuda/3.2.16
pgfortran -c m_interface.f90
pgfortran -fast -Mcuda=3.2 -lcublas m_interface.o cublas_iso_c_binding.cuf
```

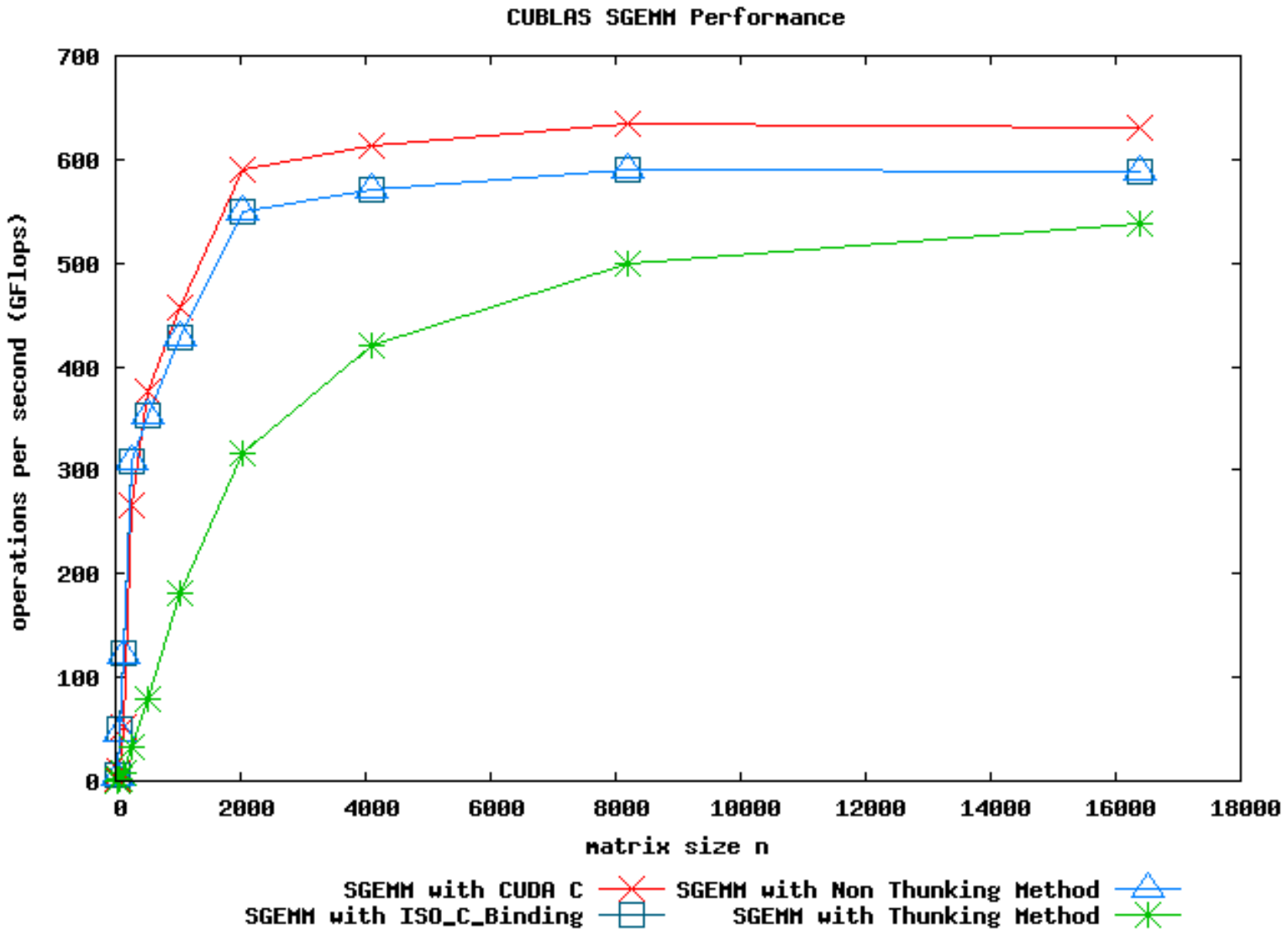
Thunking method:

```
module load compiler/pgi gpu/cuda/3.2.16
gcc -O3 -I$(CUDA_TOOLKIT)/include -c $(CUDA_TOOLKIT)/src/fortran_thunking.c
pgfortran -fast -Mcuda=3.2 -lcublas fortran_thunking.o cublas_thunking.cuf
```

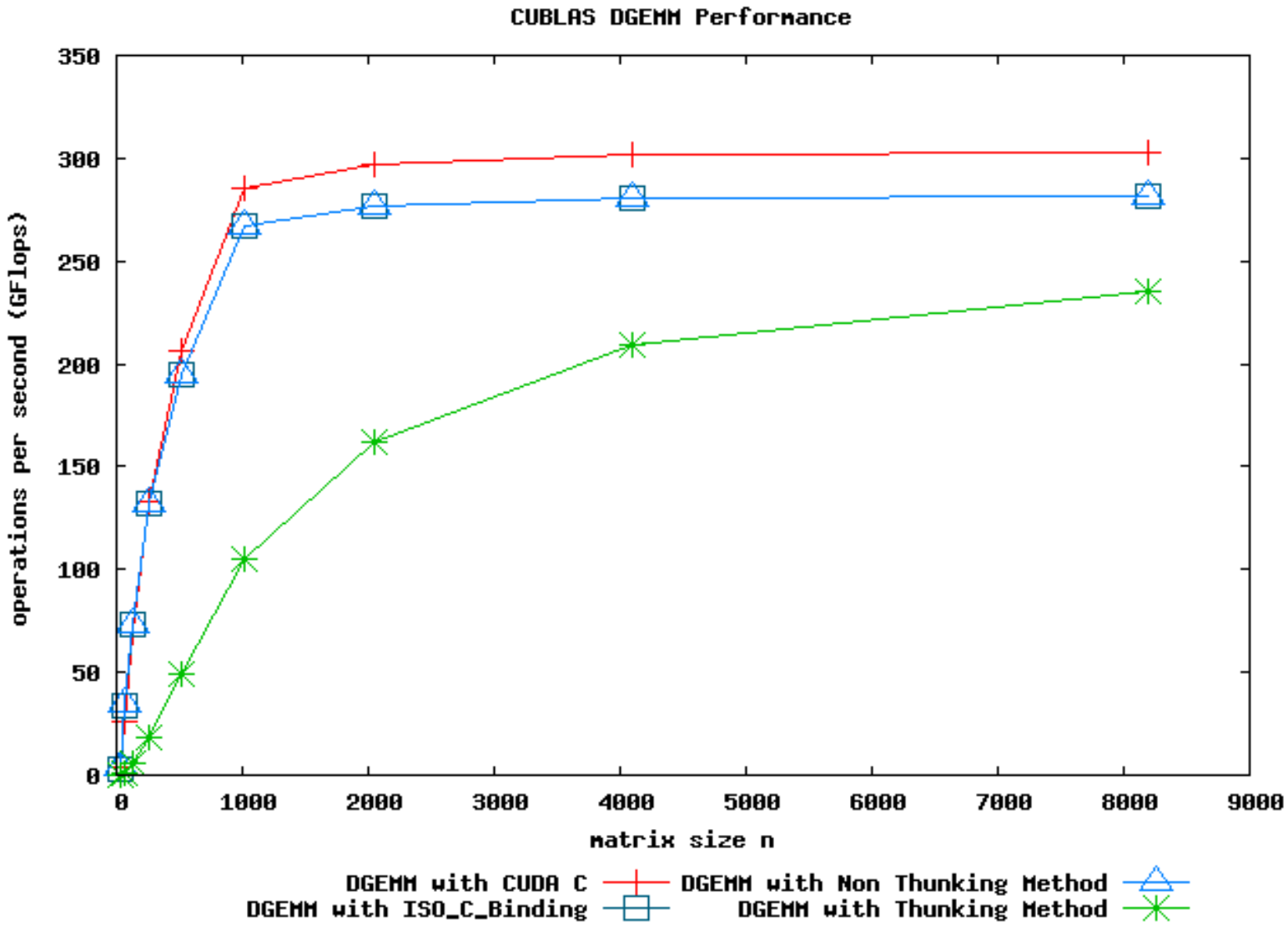
Non thunking method:

```
module load compiler/pgi gpu/cuda/3.2.16
gcc -O3 -I$(CUDA_TOOLKIT)/include -c $(CUDA_TOOLKIT)/src/fortran.c
pgfortran -fast -Mcuda=3.2 -lcublas fortran.o cublas_non_thunking.cuf
```

CUBLAS help to find performance



CUBLAS help to find performance



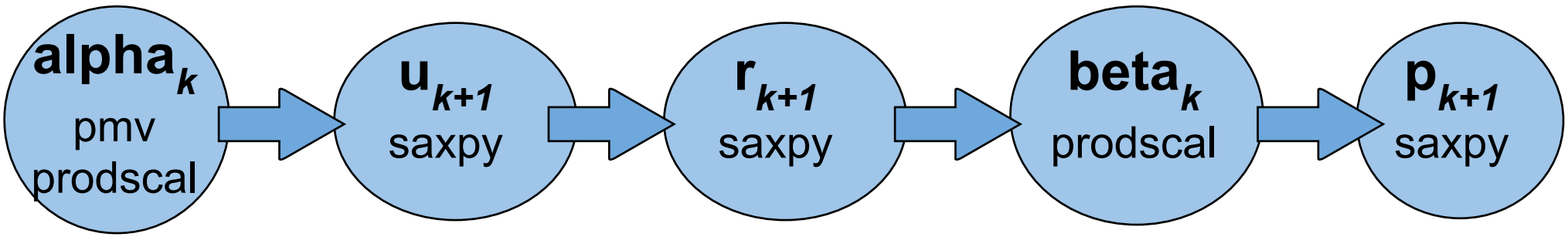
Outcome of all these sheets

- Use of libraries provides performance
  - over twice for matrix multiplication at least
- Simplify development of applications
  - focus on the integration of library calls when it is possible
  - develop kernel only if it is necessary
- Try to figure out when you have to call GPU implementation
  - bandwidth host <==> device is significant
  - give you indicators for GPU callings
- Give time to focus on optimizing other parts of program
  - profile your code to find hotspots
  - try to evaluate the necessity of GPU portability

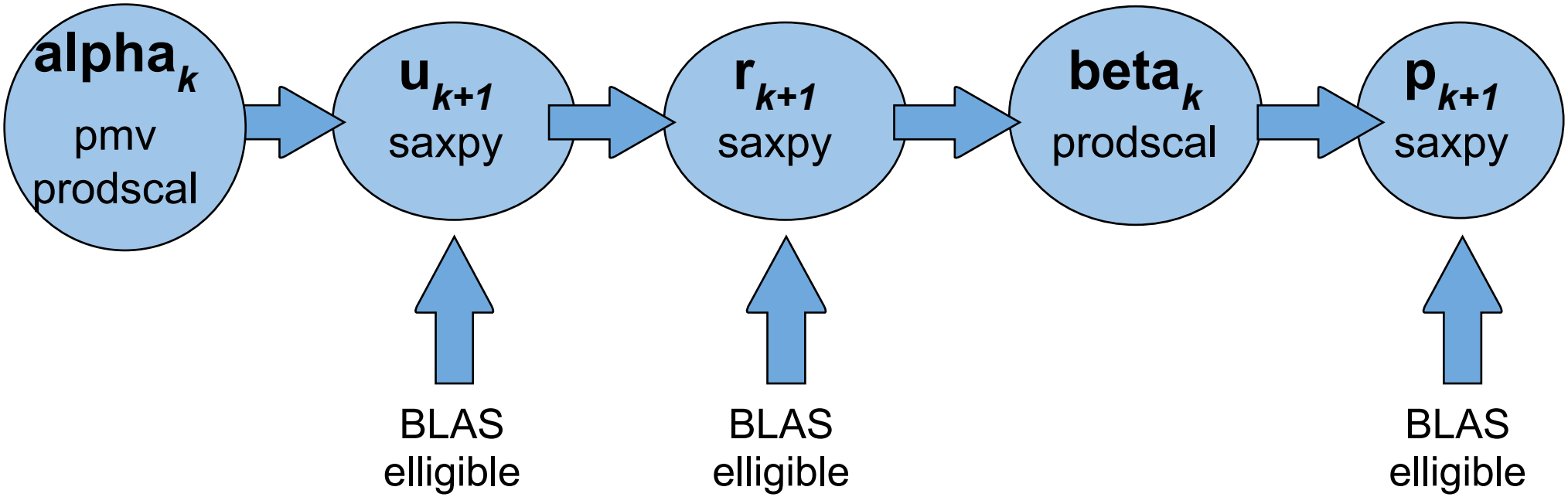
And in real life...

You have a CPU implementation

- Poisson Equation
  - conjugate gradient method
  - finite difference method
  - Jacobi solver



Find out where you can place libraries calls



Use Blas performance in this code ?

What we need to run on GPU?

```
do (it = 0 ; it < 1000 ; it ++)

   //calcul de \alpha_k
   (...)
   pmv(q,p)
   prodscal(alpha_k,q,p,comm3d)
   (...)
   //calcul de u_k+1
   saxpy( u, 1.0,  p,    alpha_k )
   //calcul de r_k+1
   saxpy( r,  1.0,  q,  - alpha_k )
   // calcul de \beta_k
   prodscal(  rnorm_k,  r,  r,  comm3d  )
   (...)
   // calcul de p_k+1
   saxpy(  p,  beta_k,  r,  1.0 )
   convergence()

enddo
```

Fortran thunking mode

→ cublas_daxpy(dimtot,alpha$_k$,p,1,u,1)

→ cublas_daxpy(dimtot,-alpha$_k$,q,1,r,1)

→ cublas_daxpy(dimtot,beta$_k$,p,1,r,1)

Outline

```
do (it = 0 ; it < 1000 ; it ++)

   //calcul de \alpha_k
   (...)
   pmv(q,p)
   prodscal(alpha_k,q,p,comm3d)
   (...)
   //calcul de u_k+1
   saxpy( u, 1.0,  p,    alpha_k )
   //calcul de r_k+1
   saxpy( r,  1.0,  q,  - alpha_k )
   // calcul de \beta_k
   prodscal(  rnorm_k,  r,  r,  comm3d  )
   (...)
   // calcul de p_k+1
   saxpy(  p,  beta_k,  r,  1.0 )
   convergence()

enddo
```

total time to compute :
- cpu implementation: 6.77 sec
- gpu implementation: 25.02 sec

Fortran thunking mode

→ cublas_daxpy(dimtot,alpha_k,p,1,u,1)

→ cublas_daxpy(dimtot,-alpha_k,q,1,r,1)

→ cublas_daxpy(dimtot,beta_k,p,1,r,1)

transfert :
11008 ko up&down
Bandwidth :
Peak perf 8Gb/s
time to transfert :
2,6 ms

added host/device bandwidth: 15,74 sec

Outlines

When going on GPU is profitable?

APPROACH	EXAMPLES
Application Integration	MATLAB, Mathematica, LabVIEW
Implicit Parallel Languages	PGI Accelerator, HMPP
Abstraction Layer/Wrapper	PyCUDA, CUDA.NET, jCUDA
Language Integration	CUDA C/C++, PGI CUDA Fortran
Low-level Device API	CUDA C/C++, DirectCompute, OpenCL

Go on GPU at your speed

- Profile your code or analyse your method
  - size of your problem
  - fine grain or coarse grain ?
  - be careful of the ratio data transfers versus kernel computation
- Needed time to have a portable code
  - often more than one year ...
  - dedicated to one kind of GPU architecture ?

- Extract some eligible kernels but ...
  - libraries do the work
  - libraries are not the solution for every problem

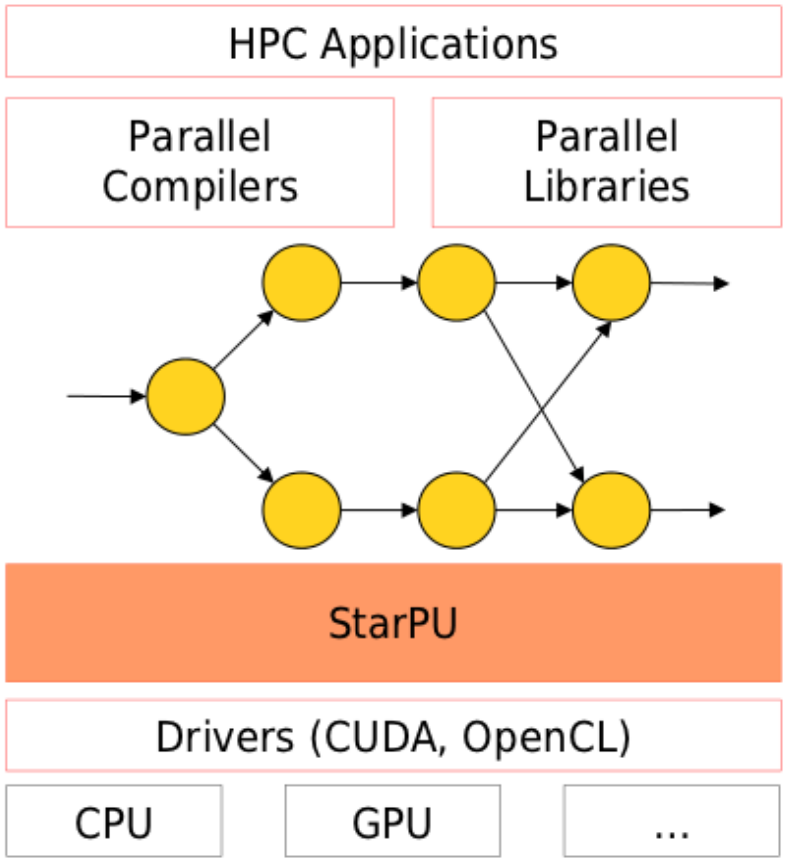
Your implementation will be portable?

- Adapt your kernels to card specifications:
  - type of memory
    - global memory,
    - shared memory,
    - texture memory...
  - size of memory
    - block size,
    - grid size...

- Choose your level
    - thunking or non-thunking
    - iso c-binding
    - low or high level API

What is your future?

- MPI + OpenMP + CUDA?
- Task scheduler and more ...
  - StarPU
  - RUNTIME Team
- PlaFRIM GT GPU :
  - gt-gpu@inria.fr
  - PlaFRIM Team



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References

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- http://tcuvelier.developpez.com/tutoriels/gpgpu/cuda/approfondi/?page=librairies