

# Tutorial on Programming GPUs

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## Abstract

The new NVIDIA Fermi GPU architecture has hardware for cache and fast native atomic operations. These features allow one to obtain decent performance with less programming effort than before. A short tutorial on programming GPUs will be presented, making use of simple examples. We will discuss the important concepts of data coalescence, warp divergence, and tiling. Examples will be presented in both Cuda Fortran and Cuda C. If time permits, we will illustrate how these ideas were applied to a Particle-in-Cell code.

## Outline of Presentation

- Abstraction of future computer hardware
- Vector copy example (segmenting problem, data coalescence)
- Transpose example (tiling with shared memory)
- Sum reduction example (device functions)

All examples are in the file GPUTutorial.tar.gz

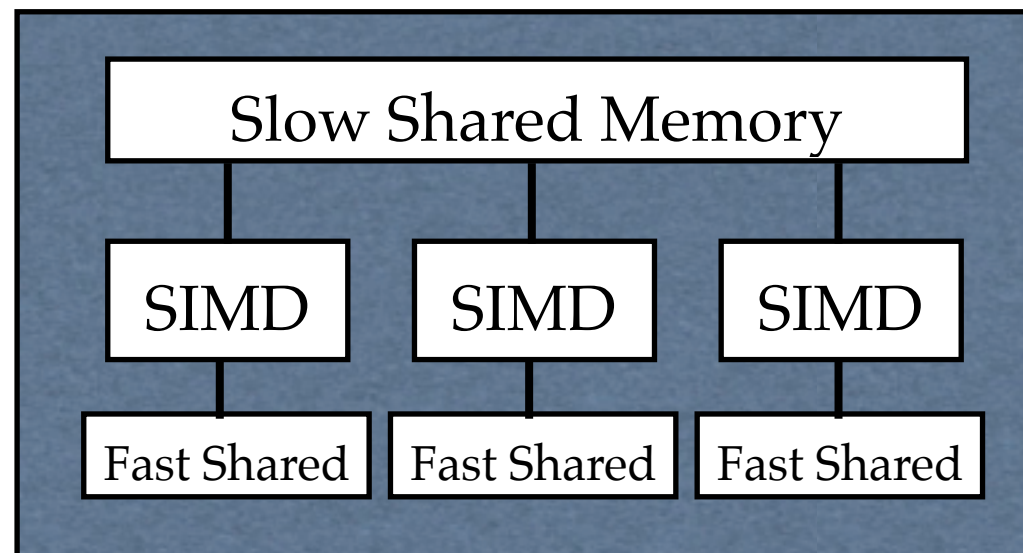
README file describes contents

There are 3 versions of each example in this file:

- Cuda C, with Fortran 90 main program
- Cuda C, with C main program
- Cuda Fortran

Cuda Fortran will be used in this presentation

## Simple abstraction of future hardware



- SIMD (vector) unit has multiple cores, each executing the same instruction
- Cores work in lockstep with fast shared memory and local synchronization
- Multiple SIMD units coupled via “slow” shared memory and global synchronization

Each compute node is a powerful computer by itself

- A supercomputer is a hierarchy of such powerful computers

This abstraction applies to both GPUs as well as upcoming multi-core Intel processors

- Programming languages generally differ, however



GPUs are graphical processing units which consist of:

- 12-30 SIMD multiprocessors, each with small (16-48KB), fast (4 clocks) shared memory
- Each multi-processor contains 8-32 processor cores
- Large (0.5-6.0 GB), slow (400-600 clocks) global shared memory, readable by all units
- No cache on some units
- **Very fast (1 clock) hardware thread switching**

GPU Technology has two special features:

- High bandwidth access to global memory (>100 GBytes/sec)
- Ability to handle thousands of threads simultaneously, greatly reducing memory “stalls”

NVIDIA M2090 has 512 cores!

# Programming GPUs

Programming Massively Parallel Processors: A Hands-on Approach  
by David B. Kirk and Wen-mei W. Hwu [Morgan Kaufmann, 2010].

CUDA by Example: An Introduction to General-Purpose GPU Programming  
Jason Sanders and Edward Kandrot [Addison-Wesley, 2011].

CUDA Application Design and Development  
by Rob Farber [Morgan Kaufmann, 2011].

CUDA Programming: A Developer's Guide to Parallel Computing with GPUs  
by Shane Cook [Morgan Kaufmann, 2012].

<http://developer.nvidia.com/cuda-downloads>

# Programming GPUs: Example 1

Let's consider a very simple example: copying one 1D array to another  
Each SIMD unit processes one block of the total problem

Original vector copy  
Parallelized with OpenMP

```
subroutine copy0(a,b)
! simple 1d copy of length nx
! a = b
  implicit none
  real, dimension(:) :: a, b
  integer :: j, nx
  nx = min(size(a,1),size(b,1))

!$OMP PARALLEL DO PRIVATE(j)
  do j = 1, nx
    a(j) = b(j)
  enddo
!$OMP END PARALLEL DO

  end subroutine
```

Stride 1 memory access important:  
Read memory locations in order

Serial segmented 1d vector copy  
Break up loops into blocks of size mx

```
subroutine copy1(a,b,mx)
! segmented 1d copy of length nx, with block size mx
! a = b
  implicit none
  integer :: mx
  real, dimension(:) :: a, b
  integer :: j, js, jb, nx, nbx

  nx = min(size(a,1),size(b,1))
  nbx = (nx - 1)/mx + 1

  do jb = 1, nbx      ! outer loop over number of blocks
    do js = 1, min(mx,nx-mx*(jb-1)) ! loop over block
      j = js + mx*(jb - 1)
      a(j) = b(j)
    enddo
  enddo

  end subroutine
```

## Programming GPUs:

### Copying one 1D array to another

Threads on each block (threadIdx) run on a single SIMD unit, execute the same instruction.

Different blocks (blockIdx) run on different SIMD units

```
subroutine copy1(a,b,mx)
! a = b
implicit none
integer :: mx
real, dimension(:) :: a, b
integer :: j, js, jb, nx, nbx

nx = min(size(a,1),size(b,1))
nbx = (nx - 1)/mx + 1

do jb = 1, nbx
  do js = 1, min(mx,nx-mx*(jb-1))
    j = js + mx*(jb - 1)
    a(j) = b(j)
  enddo
enddo

end subroutine
```

### The loop parameters set by host calling function:

```
subroutine gpu_copy1(a,b,mx)
! outer part of loop goes here
implicit none
integer :: mx, nx, nbx
real, device, dimension(:) :: a, b
type (dim3) :: dimBlock, dimGrid
nx = min(size(a,1),size(b,1))
nbx = (nx - 1)/mx + 1
dimBlock = dim3(mx,1,1)    ! size of block
dimGrid = dim3(nbx,1,1)    ! number of blocks

call gcopy1<<<dimGrid,dimBlock>>>(a,b,nx)

crc = cudaThreadSynchronize()
end subroutine
```

### The inner part of loop in GPU kernel function:

```
attributes(global) subroutine gcopy1(a,b,nx)
! inner part of loops goes here
implicit none
integer, value :: nx
real, dimension(nx) :: a, b
integer :: j, js, jb, mx
mx = blockDim%x          ! comes from dimBlock
js = threadIdx%x        ! comes from dimBlock
jb = blockIdx%x         ! comes from dimGrid

j = js + mx*(jb - 1)
if (j <= nx) a(j) = b(j)

end subroutine
```

# Programming GPUs: CUDA Fortran

In addition, you must initialize memory on the GPU

```
real, dimension(:), allocatable :: a, b
real, device, dimension(:), allocatable :: g_a, g_b
! allocate host data
allocate(a(nx),b(nx),c(nx))
! allocate data on GPU, using Fortran90 array syntax
allocate(g_a(nx),g_b(nx))
```

## Copy from host to GPU

```
! Copy data to GPU, using Fortran90 array syntax
g_b = b
```

## Execute the subroutine:

```
! Execute on GPU: g_a = g_b
call gpu_copy1(g_a,g_b,mx)
```

## Copy from GPU back to host

```
! Copy data from GPU, using Fortran90 array syntax
a = g_a
```

CUDA C is similar but more complex (no array syntax, separate memory spaces)



## Programming GPUs:

### Copying one **2D** array to another

#### Serial segmented 2d vector copy

```
subroutine copy2(a,b,mx)
! segmented 2d copy of length nx, ny
! with block size mx
! a = b
implicit none
integer :: mx
real, dimension(:, :) :: a, b
integer :: j, k, nx, ny, js, jb, nbx

nx = min(size(a,1),size(b,1))
ny = min(size(a,2),size(b,2))
nbx = (nx - 1)/mx + 1

do k = 1, ny
  do jb = 1, nbx
    do js = 1, min(mx,nx-mx*(jb-1))
      j = js + mx*(jb - 1)
      a(j,k) = b(j,k)
    enddo
  enddo
enddo

end subroutine
```

In Fortran, first index is adjacent  
in memory

## Changes to host calling function:

Each y value is a separate block, nbx\*ny blocks

```
subroutine gpu_copy2a(a,b,mx)
! outer part of loop goes here
...
real, device, dimension(:, :) :: a, b
ny = min(size(a,2),size(b,2))
dimGrid = dim3(nbx,ny,1)

call gcopy2a<<<dimGrid,dimBlock>>>(a,b,nx,ny)

...
end subroutine
```

## GPU kernel function:

```
attributes(global) subroutine gcopy2a(a,b,nx,ny)
implicit none
integer, value :: nx, ny
real, dimension(nx,ny) :: a, b
integer :: j, js, jb, k, mx
mx = blockDim%x
js = threadIdx%x
jb = blockIdx%x
k = blockIdx%y

j = js + mx*(jb - 1)
if ((j <= nx).and.(k <= ny)) a(j,k) = b(j,k)

end subroutine
```

Programming GPUs:  
Copying one 2D array to another

**Fewer blocks, more work per block**

prior GPU kernel function:

```
attributes(global) subroutine
                                gcopy2a(a,b,nx,ny)

implicit none
integer, value :: nx, ny
real, dimension(nx,ny) :: a, b
integer :: j, js, jb, k, mx
mx = blockDim%x
js = threadIdx%x
jb = blockIdx%x
k = blockIdx%y

j = js + mx*(jb - 1)
if ((j <= nx).and.(k <= ny)) then
    a(j,k) = b(j,k)
endif

end subroutine
```

Changes to host calling function:  
One block handles all x values

```
subroutine gpu_copy2b(a,b,mx)
! outer part of loop goes here
...
dimGrid = dim3(ny,1,1)

call gcopy2b<<<dimGrid,dimBlock>>>(a,b,nx,ny)

...
end subroutine
```

GPU kernel function:

```
attributes(global) subroutine gcopy2b(a,b,nx,ny)
implicit none
integer, value :: nx, ny
real, dimension(nx,ny) :: a, b
integer :: j, k, mx
mx = blockDim%x                                ! jb no longer needed
k = blockIdx%x

j = threadIdx%x
do while (j <= nx)
    if (k <= ny) a(j,k) = b(j,k)
    j = j + mx
enddo

end subroutine
```

## Programming GPUs:

### Copying one 2D array to another

#### Doubly segmented serial 2d vector copy

```
subroutine copy3(a,b,mx,my)
! segmented 2d copy of length nx, ny
! with block size mx, my
! a = b
implicit none
integer :: mx, my
real, dimension(:, :) :: a, b
integer :: j, k, nx, ny, js, ks
integer :: jb, kb, nbx, nby
nx = min(size(a,1),size(b,1))
ny = min(size(a,2),size(b,2))
nbx = (nx - 1)/mx + 1
nby = (ny - 1)/my + 1

do kb = 1, nby
do jb = 1, nbx
do ks = 1, min(my,ny-my*(kb-1))
k = ks + my*(kb - 1)
do js = 1, min(mx,nx-mx*(jb-1))
j = js + mx*(jb - 1)
a(j,k) = b(j,k)
enddo
enddo
enddo
enddo

end subroutine
```

## Changes to host calling function:

### One block handles some x,y values

```
subroutine gpu_copy3(a,b,mx)
! outer part of loop goes here
...
real, device, dimension(:, :) :: a, b
dimBlock = dim3(mx,my,1)
dimGrid = dim3(nbx,nby,1)

call gcopy3<<<dimGrid,dimBlock>>>(a,b,nx,ny)

...
end subroutine
```

### GPU kernel function:

```
attributes(global) subroutine gcopy3(a,b,nx,ny)
implicit none
integer, value :: nx, ny
real, dimension(nx,ny) :: a, b
integer :: j, k, js, ks, jb, kb, mx, my
mx = blockDim%x; my = blockDim%y
js = threadIdx%x; ks = threadIdx%y
jb = blockIdx%x; kb = blockIdx%y

k = ks + my*(kb - 1)
j = js + mx*(jb - 1)
if ((j <= nx) .and. (k <= ny)) a(j,k) = b(j,k)

end subroutine
```

# Programming GPUs: Vector copy

## Summary

- Processing must be segmented into independent blocks
- Inner loop runs on GPU, loop parameters are set on host
- Data coalescing is important (adjacent threads read adjacent memory locations)
- Each block should execute same instruction (avoid complex if statements)

# Programming GPUs: CUDA Fortran

Sample output:

```
make cudaf
```

```
./fexample1
```

```
j=      0 :CUDA_DEVICE_NAME=Tesla M2090
  CUDA_MULTIPROCESSOR_COUNT=      16
  CUDA_GLOBAL_MEM_SIZE=      5636554752 (  5.249451  GB)
  Capability=      20
using device j=      0
Fortran empty kernel time=  2.2300000E-04
Fortran 1d copy time=  3.0000001E-06
GPU 1d copy time=  7.4000003E-05
1d copy maximum difference =  0.000000
Fortran 2d copy time=  3.6940000E-03
GPU 2d copy time=  4.3499999E-04
2d copy maximum difference =  0.000000
```

Homework: vary blocksize mx and data lengths nx, ny



# Programming GPUs: Transpose 2D array

On GPU,  $mx = my$

```
subroutine transpose2(a,b,mx,my)
! a = transpose(b)
...
real, dimension(mx+1,my) :: s
...
do kb = 1, nby
  koff = my*(kb - 1)
  do jb = 1, nbx
    joff = mx*(jb - 1)
    do ks = 1, min(my,ny-koff)
      k = ks + koff
      do js = 1, min(mx,nx-joff)
        j = js + joff
        s(js,ks) = b(j,k)
      enddo
    enddo
  enddo
do js = 1, min(mx,nx-joff)
  j = js + joff
  do ks = 1, min(my,ny-koff)
    k = ks + koff
    a(k,j) = s(js,ks)
  enddo
enddo
enddo
enddo
end subroutine
```

The inner part of loop in GPU kernel function:

```
attributes(global) subroutine
                                gtranspose2(a,b,nx,ny)
! inner part of loops go here
implicit none
integer, value :: nx, ny
real, dimension(ny,nx) :: a
real, dimension(nx,ny) :: b
integer :: j, k, js, ks, jb, kb
integer :: joff, koff, mx, mxv
real, shared, dimension(*) :: s
mx = blockDim%x; mxv = mx + 1
js = threadIdx%x; ks = threadIdx%y
jb = blockIdx%x; kb = blockIdx%y
koff = mx*(kb - 1)
joff = mx*(jb - 1)

k = ks + koff
j = js + joff
if ((j <= nx) .and. (k <= ny)) then
  s(js+mxv*(ks-1)) = b(j,k)
endif

call syncthreads() ! synchronize threads

j = ks + joff
k = js + koff
if ((j <= nx) .and. (k <= ny)) then
  a(k,j) = s(ks+mxv*(js-1))
endif
end subroutine
```

# Programming GPUs: Transpose 2D array

## GPU kernel function:

```
attributes(global) subroutine
    gtranspose2(a,b,nx,ny)

...
real, shared, dimension(*) :: s
mx = blockDim%x; mxv = mx + 1
js = threadIdx%x; ks = threadIdx%y
jb = blockIdx%x; kb = blockIdx%y
koff = mx*(kb - 1)
joff = mx*(jb - 1)

k = ks + koff
j = js + joff
if ((j <= nx).and.(k <= ny)) then
    s(js+mxv*(ks-1)) = b(j,k)
endif

call syncthreads()

j = ks + joff
k = js + koff
if ((j <= nx).and.(k <= ny)) then
    a(k,j) = s(ks+mxv*(js-1))
endif
end subroutine
```

## Host calling function similar to gpu\_copy3

```
subroutine gpu_transpose2(a,b,mx)
...
real, device, dimension(:,:) :: a, b
...
dimBlock = dim3(mx,mx,1)
dimGrid = dim3(nbx,nby,1)
! calculate size of shared memory
ns = (mx + 1)*mx*sizeof(a(1,1))

call gtranspose2<<<dimGrid,dimBlock,ns>>>(a,b,nx,ny)

crc = cudaThreadSynchronize()

end subroutine
```



# Programming GPUs: Transpose

## Summary

- Stride 1 access is obtained to slow global memory
- Stride 1 access is not obtained to fast shared memory, but it is 100x faster
- Processing in pieces small enough to fit in fast memory (tiling) is important

# Programming GPUs: CUDA Fortran

Sample output:

```
./fexample2
```

```
using device j=      0
Fortran empty kernel time=  2.2800000E-04
Fortran 2d transpose time=  4.2500001E-04
GPU 2d transpose time=  2.5099999E-04
2d transpose maximum difference =  0.000000
```

# Programming GPUs: Example 3

## Sum reduction of 1D array

### Original sum reduction

### Parallelized with OpenMP

```
subroutine sum0(a,sa)
! simple 1d sum reduction of length nx
! sa = sum(a)
  implicit none
  real :: sa
  real, dimension(:) :: a
  integer :: j

  sa = 0.0
!$OMP PARALLEL DO PRIVATE(j)
!$OMP& REDUCTION(+:sa)
  do j = 1, size(a,1)
    sa = sa + a(j)
  enddo
!$OMP END PARALLEL DO
end subroutine
```

Stride 1 memory access important:  
Read memory locations in order

### Serial segmented 1d sum reduction

### Partial sums of blocks of size mx

```
subroutine sum1(a,sa,mx)
! 1d sum reductions, each of length mx
! sa = sum(a)
  implicit none
  integer :: mx
  real :: sa
  real, dimension(:) :: a
  integer :: j, js, jb, nx, nbx
  real :: t
  nx = size(a,1)
  nbx = (nx - 1)/mx + 1

  sa = 0.0
  do jb = 1, nbx
    t = 0.0
    do js = 1, min(mx,nx-mx*(jb-1))
      j = js + mx*(jb - 1)
      t = t + a(j)
    enddo
    sa = sa + t

  enddo

end subroutine
```

# Programming GPUs:

## Sum reduction of 1D array

On GPU, copy to shared memory  
one thread performs partial sum  
Not very efficient

```
subroutine sum1(a,sa,mx)
! sa = sum(a)
...
real :: sa
real, dimension(:) :: a
...
sa = 0.0
do jb = 1, nbx
  t = 0.0
  do js = 1, min(mx,nx-mx*(jb-1))
    j = js + mx*(jb - 1)
    t = t + a(j)
  enddo
  sa = sa + t
enddo

end subroutine
```

The inner part of loop in GPU kernel function:

```
attributes(global) subroutine gsum1(a,sa,nx)
! inner part of loop goes here
implicit none
integer, value :: nx
real, dimension(:) :: a, sa
integer :: j, js, jb, mx, joff, mxm
real :: t
real, shared, dimension(*) :: s
mx = blockDim%x
js = threadIdx%x
jb = blockIdx%x
joff = mx*(jb - 1)

j = js + joff ! first copy to shared memory
if (j <= nx) s(js) = a(j)
call syncthreads()
if (js==1) then ! one thread performs sum
  mxm = nx - joff
  if (mxm > mx) mxm = mx
  t = 0.0
  do j = 1, mxm
    t = t + s(j)
  enddo
  ! sum different blocks
  t = atomicAdd(sa(1),t)
endif

end subroutine
```

# Programming GPUs:

## Sum reduction of 1D array

### GPU kernel function:

```
attributes(global) subroutine
    gsum1(a,sa,nx)

...
real, shared, dimension(*) :: s
mx = blockDim%x
js = threadIdx%x
jb = blockIdx%x
joff = mx*(jb - 1)

j = js + joff
if (j <= nx) s(js) = a(j)
call syncthreads()
if (js==1) then          mxm = nx - joff
    if (mxm > mx) mxm = mx
    t = 0.0
    do j = 1, mxm
        t = t + s(j)
    enddo
    t = atomicAdd(sa(1),t)
endif

end subroutine
```

### host calling function:

```
subroutine gpu_sum1(a,sa,mx)
implicit none
integer :: mx
real, device, dimension(:) :: a, sa
integer :: nx, nbx, ns
type (dim3) :: dimBlock, dimGrid
nx = size(a,1)
nbx = (nx - 1)/mx + 1
dimBlock = dim3(mx,1,1)
dimGrid = dim3(nbx,1,1)
sa(1) = 0.0
! calculate size of shared memory
ns = mx*sizeof(a(1))

call gsum1<<<dimGrid,dimBlock,ns>>>(a,sa,nx)

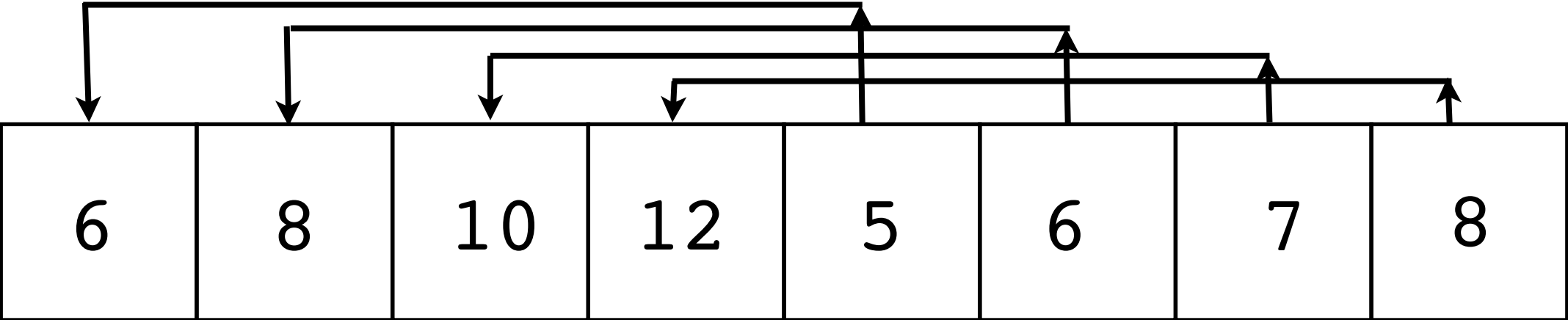
end subroutine
```

Parallel Sum Reduction:

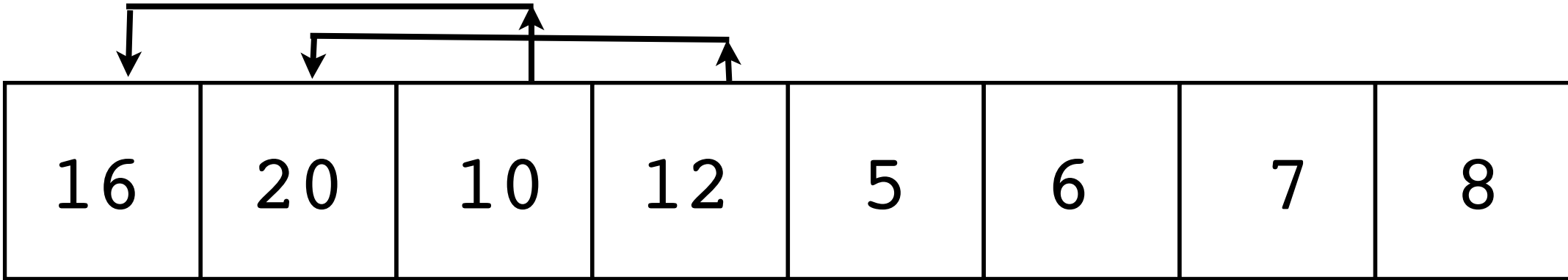
0:

1	2	3	4	5	6	7	8
---	---	---	---	---	---	---	---

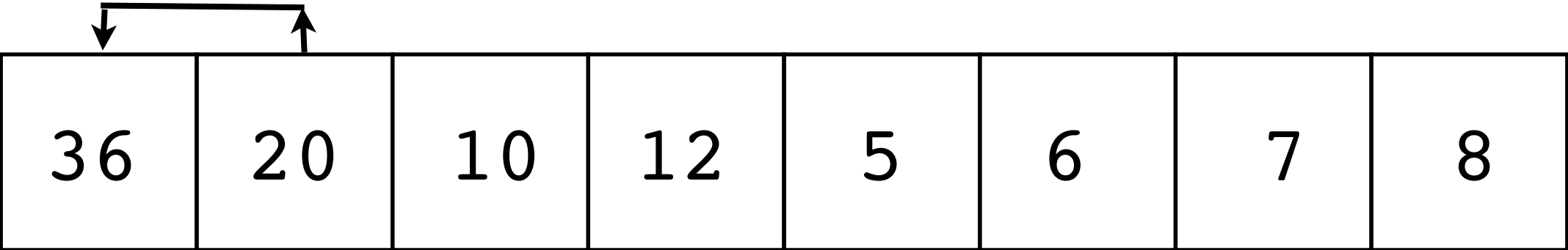
1:



2:



3:



# Programming GPUs: Sum reduction of 1D array

Implementation of local parallel sum reduction  
device functions are inlined, sdata is in shared memory

```
attributes(device) subroutine lsum2(sdata,n)
! finds local sum of n data items shared by threads
! using binary tree method. input is modified
  implicit none
  real, dimension(*) :: sdata
  integer, value :: n
  integer :: l, k
  real :: s
  l = threadIdx%x
  k = blockDim%x/2
  s = 0.0

  if (l <= n) s = sdata(l)
  do while (k > 0)
    if (l <= k) then
      if ((l+k) <= n) then
        s = s + sdata(l+k)
        sdata(l) = s
      endif
    endif
    call syncthreads()
    k = k/2
  enddo

end subroutine
```

## Programming GPUs:

### Sum reduction of 1D array

Prior GPU kernel function:

```
attributes(global) subroutine
    gsum1(a,sa,nx)
...
real, shared, dimension(*) :: s
mx = blockDim%x
js = threadIdx%x
jb = blockIdx%x
joff = mx*(jb - 1)

j = js + joff
if (j <= nx) s(js) = a(j)
call syncthreads()

if (js==1) then
    mxm = nx - joff
    if (mxm > mx) mxm = mx
    t = 0.0
    do j = 1, mxm
        t = t + s(j)
    enddo
    t = atomicAdd(sa(1),t)
endif

end subroutine
```

Multiple parallel sum reductions:  
**write out partial sum of each block**

GPU kernel function:

```
attributes(global) subroutine gsum2(a,d,nx)
implicit none
integer, value :: nx
real, dimension(:) :: a, d
integer :: j, js, jb, mx, joff, mxm
real, shared, dimension(*) :: s
mx = blockDim%x
js = threadIdx%x
jb = blockIdx%x
joff = mx*(jb - 1)

j = js + joff
if (j <= nx) s(js) = a(j)
call syncthreads()

mxm = nx - joff
if (mxm > mx) mxm = mx
call lsum2(s,mxm)
if (js==1) d(jb) = s(1)

end subroutine
```



## Programming GPUs: Sum reduction of 1D array

### GPU kernel function:

```
attributes(global) subroutine
    gsum2(a,d,nx)
implicit none
integer, value :: nx
real, dimension(:) :: a, d
integer :: j, js, jb, mx, joff, mxm
real, shared, dimension(*) :: s
mx = blockDim%x
js = threadIdx%x
jb = blockIdx%x
joff = mx*(jb - 1)

j = js + joff
if (j <= nx) s(js) = a(j)
call syncthreads()

mxm = nx - joff
if (mxm > mx) mxm = mx
call lsum2(s,mxm)
if (js==1) d(jb) = s(1)

end subroutine
```

Multiple parallel sum reductions:  
write out partial sum of each block

### host calling function:

```
subroutine gpu_sum2(a,d,mx)
implicit none
integer :: mx
real, device, dimension(:) :: a, d
integer :: nx, nbx, ns
type (dim3) :: dimBlock, dimGrid
nx = size(a,1)
nbx = (nx - 1)/mx + 1
dimBlock = dim3(mx,1,1)
dimGrid = dim3(nbx,1,1)
! calculate size of shared memory
ns = mx*sizeof(a(1))

call gsum2<<<dimGrid,dimBlock,ns>>>(a,d,nx)

crc = cudaThreadSynchronize()

end subroutine
```

## Programming GPUs: Sum reduction of 1D array

Many times only local sums are required

If global sum is needed, one can combine these two procedures

Perform parallel sums for each block:

```
call gpu_sum2(g_a,g_d,mx)
```

Then add the partial sums with serial algorithm:

```
call gpu_sum1(g_d,g_s,mx)
```

If array is long, one can iterate `gpu_sum2` several times.

This is done by the host procedure `gpu_sum3`:

```
call gpu_sum3(g_a,g_d,g_s,mx)
```

Sample output:

```
./fexample3
```

```
Fortran empty kernel time= 5.1999999E-05
```

```
Fortran 1d sum time= 4.0000000E-06
```

```
GPU 1d sum time= 2.5300001E-04
```

```
1d sum maximum difference = 0.000000
```

```
s,t = 4501500. 4501500.
```

## Programming GPUs: Conclusions

- Vector algorithms are relatively easy
- Processing has to be done in small blocks
- Tiling algorithms are well known from cache based machines
- Sum reductions are harder
- Irregular problems such as reordering data can be very hard
- Very useful to develop a serial version before implementing a Cuda version
- Libraries such as BLAS, FFTs, are available to avoid reinventing the wheel
- New languages such as OpenACC (similar to OpenMP) are evolving