Use of Accelerate Tools
PGI CUDA FORTRAN
Jacket

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Tentative Agenda:

9:30 -10:00 Intro – GPU computing, Hardware (Jeff)
10:00 -11:00 Basics of Cuda Programming (Weijun)
11:00 -12:00 hands-on exercise

1:00 - 1:40 Use of Memory Hierarchy for Performance Enhancement (David)
1:50 – 2:10 hands-on exercise
2:10 – 2:20 Break
2:20 – 3:10 Use of acceleration tools (Shuxia)
CUDA FORTRAN & Jacket
3:10 – 4:00 hands-on exercises

Survey Questionaires:

Why are you interested in GPU computing?

What kind of applications do you need to accelerate on GPU hardware?

Do you have the computing code(s) already on CPU?
If yes, in what language is it written (C, FORTRAN or Matlab)?

Do you have a deadline or milestone to get your computing on GPU hardware? When?

Specific need about the hardware (memory, mutli-GPU and interconnect need)?

Will you learn CUDA or use the acceleration tools to get your calculations on GPU hardware?

How can we do better for the future GPU workshop:
Specific topics are you interested?
Specific acceleration tools?

PGI CUDA FORTRAN

1. A small set of extensions to Fortran
2. Supports and is built up on the CUDA
3. A lower-level explicit programming model
4. Substantial run-time library components
5. An analog to NVIDIA's CUDA C compiler

Portland License!

CUDA Fortran extensions :

- Declaring variables allocated in the GPU device memory
- Allocating dynamic memory in the GPU device memory
- Copying data between the host memory to the GPU memory
- Writing subroutines and functions to execute on the GPU
- Invoking GPU subroutines from the host
- Allocating pinned memory on the host
- Using asynchronous transfers between the host and GPU

CUDA Fortran Programming

- Host code
  - Optional: select a GPU
  - Allocate device memory
  - Copy data to device memory
  - Launch kernel(s)
  - Copy data from device memory
  - Deallocate device memory
- Kernel code
  - Attributes clause
  - Kernel subroutines, device subprograms
  - Shared memory
  - What is and what is not allowed in a kernel

CUDA C vs CUDA Fortran

CUDA C
- supports texture memory
- supports Runtime API
- supports Driver API
- cudaMalloc, cudaFree
- cudaMemcpy
- OpenGL interoperability
- Direct3D interoperability
- arrays zero-based
- threadidx/blockidx 0-based
- unbound pointers
- pinned allocate routines

CUDA Fortran
- no texture memory
- supports Runtime API
- no support for Driver API
- allocate, deallocate
- Assignments (A=d)A
- no OpenGL interoperability
- no Direct3D interoperability
- arrays one-based
- threadidx/blockidx 1-based
- allocatable are device/host
- pinned attribute

CUDA Fortran Programming

Key building blocks:

- Use the cudafor module
- Attributes clause
- Kernel subroutines, device subprograms
- Use of memory hierarchy
- Thread Blocks
- What is and what is not allowed in a kernel

Intrinsic data-types in device subprograms

Type	Type Kind
integer	1,2,4,8
logical	1,2,4,8
real	4,8
double precision	real(kind=8)

CUDA Fortran Programming

- Host code – GPU-related operations
  - Optional: select a GPU
  - Allocate device memory
  - Copy data to device memory
  - Launch kernel(s)
  - Copy data from device memory
  - Deallocate device memory
- Device code
  - Scalar thread code, limited operations
  - Implicitly parallel
    - thread blocks scheduled by hardware on any multiprocessor
    - runs to completion before next kernel

```fortran
subroutine vadd( A, B, C )
use kmod
real(4), dimension(:) :: A, B, C
real(4), device, allocatable, &
dimension(:):: Ad, Bd, Cd
integer :: N
N = size( A, 1 )
allocate( Ad(N), Bd(N), Cd(N) )
Ad = A(1:N)
Bd= B(1:N)
!call kernel<<< grid, block >>>( Ad, Bd, Cd, N )
call kernel<<< (N+31)/32, 32 >>>( Ad, Bd, Cd, N )
C(1:N) = Cd
deallocate(Ad, Bd, Cd)
end subroutine
```

```fortran
subroutine vadd(A,B,C,N)
real(4) :: A(N), B(N), C(N)
integer :: N
integer :: i
do i = 1,N
C(i) = A(i) + B(i)
enddo
end subroutine
```

```
module kmod
 use cudafor
contains
 attributes(global) subroutine kernel(A,B,C,N)
  real(4), device :: A(N), B(N), C(N)
  integer, value :: N
  integer :: i
  i = (blockidx%x-1)*32 + threadidx%x
  if( i <= N ) C(i) = A(i) + B(I)
 end subroutine
end module
```

global means kernel

device attribute implied

value vs. Fortran default

blockidx from 1..(N+31)/32

threadidx from 1..32

array bounds test

Attributes clause for subroutines and/or functions

- attributes(host), or by default, host subprogram
  - to be executed on host
  - can only be called from another host subprogram
- attributes(global) - a kernel subroutine
  - to be executed on the device
  - may only be called from the host using a kernel call.
- attributes(device) - a device Subprogram, subroutine or function
  - to be executed on the device;
  - must be called from a subprogram with the global or device Attribute.

Restrictions

not be recursive, not contain variables with the save or data initialization; may not also have the device or host attribute; not have optional arguments; must not have the pointer attribute.

Attributes clause for variables and arrays

attributes(device) - device variable
allocated in the device global array

attributes(constant) – device constant variable
allocated in the device constant memory space

attributes(shared) - a device shared variable
may only be declared in a device subprogram
is allocated in the device shared memory for a thread block
can be read or written by all threads in the block

attributes(pinned) - a pinned variable
must be an allocatable array
will be allocated in host pagelocked memory

Execution Configuration

Call kernel<<<grid,block>>>(arg1,arg2,...)

Where grid and block – execution configuration

integer expression or type(dim3).

Predifined variables of type(dim3) used on host:

block – block%x, block%y, block%z

grid – grid%x, grid%y, grid%z

Predifined variables of type(dim3) used on device:

threadidx – threadidx%x,threadidx%y, threadidx%z

blockidx – blockidx%x,blockidx%y, blockidx%z

blockdim – blockdim%x,blockdim%y,blockdim%z

Asynchronous Concurrent Execution

Asynchronous Concurrent Execution

Concurrent Host and Device Execution - a kernel launch

call cudaThreadSynchronize !the host program can
synchronize and wait for all previously
launched or queued kernels

Concurrent Stream Execution

Operations involving the device, including kernel execution and data copies to and from device memory, are implemented using stream queues.

call syncthreads() ! The device program

Hands-on Exercise: https://www-test2.msi.umn.edu/content/gpu-hands-tutorial

Use of CUDA blas library

Assignment: Modify the code CPU_Sgemm.f90 to call sgemm of cuda blas library for calculating

$$C = a * A * B + b * C$$

Hints: 1.) Compile and run CPU_Sgemm as is for N =10000 to see many Gflops it achives;

2). Add the following as device interface

Get the tar file

www.msi.umn.edu/~szhang/GPU_Tools.tar

cat README

Hands-on Exercise:

```
program test_CPU_Sgemm
real, allocatable, dimension(:,:) :: a, b, c
!real, device, allocatable, dimension(:,:) :: dA, dB, dC
real :: alpha = 1.0e0
real :: beta  = 1.0e0
print *, "Enter N: "
read(5,*) n

allocate(a(n,n), b(n,n), c(n,n))
a = 2.0e0;b = 1.5e0; c = -9.9e0
!allocate (dA(n,n), dB(n,n), dC(n,n))
!dA = a; dB = b: dC = c
call sgemm('n','n', n, n, n, alpha, a, n, b, n, beta, c, n)
!call sgemm('n','n', n, n, n, alpha, dA, n, dB, n, beta, dC, n)
!c=dC
end
```

Hands-on Exercise:

How to compile

module load pgi

pgfortran -O2 -o CPU_perf CPU_Sgemm.F90 -lblas (or -lacml)

pgfortran -Mcuda -o GPU_perf GPU_Sgemm.F90 -lcublas

pgfortran -o GPU_perf GPU_Sgemm.cuf -lcublas

How to run

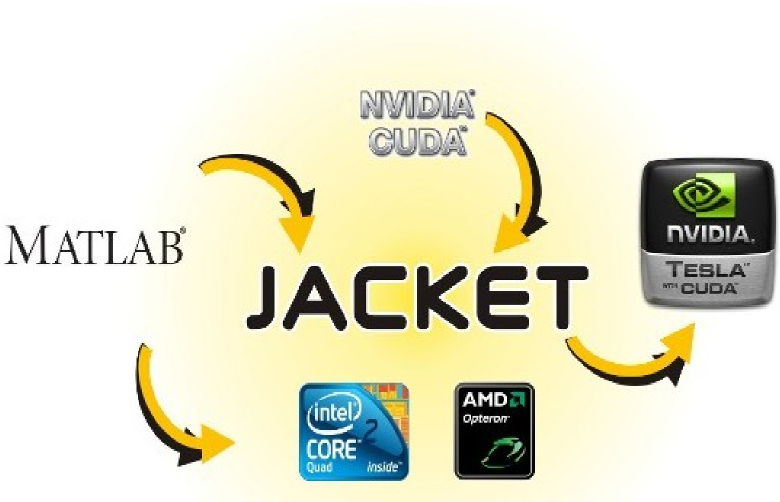
/usr/bin/time ./CPU_perf < input

/usr/bin/time ./GPU_perf < input

Jacket

Wraps some of Matlab codes
for enhancing their performance
by running on GPU

```
module load jacket matlab
matlab
>> gactivate
>> ghelp  % list all functions supported by Jacket
>> ghelp  try  %
```



All Jacket functions may be found at:
http://wiki.accelereyes.com/wiki/index.php/Function_List

How can Jacket help?

Partial support - Not every Matlab calculation can benefit

Hot spot – part of the code consumes most of the CPU time

Special functions and toolbox – are they being used? Are they supported by Jacket?

If yes, modify the code according to Jacket's syntax.

Performance Enhancement of Matlab Calculations

Use of Jacket

- replacement of low-level MATLAB data structures
- GPU computation and acceleration

Jacket Function	Description	Example
GSINGLE	Casts a CPU matrix to a single precision floating point GPU matrix.	`A = gsingle(B);`
GDOUBLE	Casts a CPU matrix to a double precision floating point GPU matrix.	`A = gdouble(B);`
GLOGICAL	Casts a CPU matrix to a binary GPU matrix. All non zero values are set to '1'. The input matrix can be a GPU or CPU datatype.	`A = glogical(B);` `A = glogical(0:4);`
GINT8, GUINT8, GINT32, GUINT32	Cast a CPU matrix to a signed and unsigned 8-bit or 32-bit integer GPU matrix respectively.	`A = gint8(B); A = guint8(B);` `A = gint32(B); A = guint32(B);`
GZEROS, ZEROS	Create a matrix of zeros on the GPU.	`A = gzeros(5,'double');` `A = zeros(2,6,gdouble);`
GONES, ONES	Create a matrix of ones on the GPU.	`A = gones(5,'double');` `A = ones([3 9], gdouble);`
GEYE	Creates an identity matrix on the GPU.	`A = geye(5);`
GRAND or RAND	Creates a random matrix on the GPU, with uniformly distributed pseudorandom numbers.	`A = grand(5,'double');` `A = rand(5,gdouble);`
GRANDN	Creates a random matrix on the GPU, with normally distributed pseudorandom numbers.	`A = grandn(5,'double');` `A = randn(5,gdouble);`

Basic functions

Jacket Function	Description	Example
GHELP	Retrieve information on the Jacket support for any function.	`ghelp sum;`
GACTIVATE	Used for manual activation of a Jacket license.	`gactivate;`
GSELECT	Select or query which GPU is in use.	`gselect(0);`

GFOR	Executes FOR loop in parallel on GPU.	`gfor n = 1:10;`
		`% loop body`
		`gend;`

GCOMPILE	Compile M-code directly into a single CUDA kernel.	`my_fn = gcompile('filename.m');` `[B C ...] = my_fn(A)`
GPROFILE	Profile code to compare CPU versus GPU runtimes.	`gprofile on; foo; gprofile off;` `gprofile report;`
GPROFVIEW	Visual representation of profiling data.	`gprofview;`
GEVAL	Evaluate computation and leave results on GPU.	`geval;`
GSYNC	Block until all queued GPU computation is complete.	`gsync(A);`
GCACHE	Save GPU compiled code for given script.	`gcache;`
GLOAD	Load from disk directly into the GPU. Requires the Jacket SDK.	`gload('filename');`
GSAVE	Save data to disk as text file directly from the GPU. Requires the Jacket SDK.	`gsave('filename', A);`
GREAD	Load from disk directly into the GPU, with option to specify the byte range. Requires the Jacket SDK.	`gread('filename', OFFSET, BYTES);`
GWRITE S	Save data to disk directly from the GPU, with option to specify the byte range. Requires the Jacket SDK.	`Gw rite('filename', OFFSET, DATA);`
Graphics	Library Functions contained in the Graphics Library.	`gplot(A);`

Find the hotspot of your code

mlint - Check M-files for possible problems

```
>> mlint lengthofline.m  % Display to command line
>> info = mlint('lengthofline') % Store to struct
```

tic/toc - accurate timing of each operation/function

```
>> tic; a=rand(1000); toc;
```

Matlab Profiler - find where the bottle neck is

```
>> profile on
>> calcultion;
>> profile off
>> profile report
```

http://www.mathworks.com/contest/protein.cgi/jitstory.html

Jacket examples:

```
Nx = 20;
n = 20;
Df = zeros(n,Nx);
X = ones(n, Nx);
for ii = 1:Nx
  Df(1,ii) = X(1,ii);
  Df(2,ii) = X(2,ii);
end
-------------------------
Option1:
Nx =20; n=20;
Df = gzeros(n,Nx);
for ii = 1:Nx
  Df(1,ii) = X(1,ii);
  Df(2,ii) = X(2,ii);
end
```

```
Option 2
Nx =20; n=20;
Df = gzeros(n,Nx);
gfor ii = 1:Nx
  Df(1,ii) = X(1,ii);
  Df(2,ii) = X(2,ii);
gend
```

Jacket examples: gfor

```
   A = gones(n,n,m);
   B = gones(n);
gfor k = 1:2:m
  A(:,:,k) = k*B + sin(k+1);  % expressions
Gend
-------------------------------------------
   A = gones(n,2*m);
   B = gones(n,m);
gfor k = 2:m
  B(:,k) = A(:,floor(k+.2));
Gend
--------------------------------------------
```

Jacket examples: fft

```
N = 128*2; % matrix size
M = 256; % number of tiled matrices
%Create Data
tic
[Ac Bc]= ...
deal(complex(ones(N,N,M,'single'),0));
toc
% Compute 200 (128x128) FFTs
tic
for ii = 1:M
   Ac(:,:,ii) = fft2(Bc(:,:,ii));
  end
Toc
%Elapsed time
%Elapsed time .
```

```
N = 128*2; % matrix size
M = 256; % number of tiled matrices
%Create Data
gsync;tic
  [Ac Bc] =
deal(complex( gones(N,N,M,'single'),0));
gsync; toc
% Compute 256 (128x128) FFTs
gsync; tic
  for ii = 1:M
  Ac(:,:,ii) = fft2(Bc(:,:,ii));
  end
gsync; toc
%Elapsed time
%Elapsed time
```

Restriction of gfor

- Iteration independence
- No conditional statements
- No cell array assignment
- Iterator not allowed in colon expressions

http://wiki.accelereyes.com/wiki/index.php/GFOR_Usage

Hands-on Exercise:

Get the tar file

www.msi.umn.edu/~szhang/GPU_Tools.tar

Tar -xvf GPU_Tools.tar
module load jacket
Matlab &
On matlab window
<< fft_cpu
<< fft-gpu

References:

http://www.pgroup.com/doc/pgicudaforug.pdf
http://www.accelereyes.com/support/documentation
http://wiki.accelereyes.com/wiki/index.php/GFOR_Usage

Need help?

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