N-WAYS GPU BOOTCAMP

STANDARD LANGUAGES

STANDARD LANGUAGES

What to expect?

- C++ , Fortran ISO standard brief
- C++ std::par , Fortran DO-Concurrent API
- Known limitations

QUICK BACKGROUND

C++ STL Containers

- One driving feature of C++ are its templates and the STL library. C++11 is further pushing these ideas and shows no sign of slowing.
- C++ templates are probably most widely used through the STL containers.
    - std::vector, std::string, std::map, std::list, etc...
- Besides the OO features and convenience, these containers are designed to rise-above basic C pointers, providing more safety from memory violations, while maintaining the bare-metal performance.
- For example std::vector ¤ The vector template is designed to replace C's arrays.

```
std::vector<int> my_ints(4, 100);   // four ints with value 100
```


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STD::PAR

What is std::par?

- Use standard C++ constructs to make code run parallel on heterogeneous hardware
- C++11 introduced a memory model, concurrent execution model, and concurrency library, providing a standard way to take advantage of multicore processors
- The C++17 Standard introduced higher-level parallelism features that allow users to request parallelization of Standard Library algorithms.

Advantage:

- No language extensions, pragmas, directives, or non-standard libraries
- Write Standard C++, which is portable to other compilers and systems
- Compiler automatically accelerates code with high-performance NVIDIA GPUs and hence less time porting and more time on what really matters

STD::PAR

Parallelism in Standard C++

- Parallelism is expressed by adding an execution policy as the first parameter to any algorithm that supports execution policies
- Most of the existing Standard C++ algorithms were enhanced to support execution policies

Execution policies can be applied to most standard algorithms

- std::execution::seq = sequential: Sequential execution. No parallelism is allowed.
- std::execution::par = parallel: Parallel execution on one or more threads.
- std::execution::par_unseq = parallel + vectorized: Parallel execution on one or more threads, with each thread possibly vectorized.

C++17 PARALLEL ALGORITHMS

Example

C++98: `std::sort(c.begin(), c.end());`

C++17: `std::sort(std::execution::par, c.begin(), c.end());`

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BUILD AND RUN THE CODE

NVIDIA HPC SDK

- Comprehensive suite of compilers, libraries, and tools used to GPU accelerate HPC modeling and simulation application
- The NVIDIA HPC SDK includes the new NVIDIA HPC C++ compiler, NVC++. NVC++ supports C++17, C++ Standard Parallelism (stdpar) for CPU and GPU
- NVC++ can compile Standard C++ algorithms with the parallel execution policies std::execution::par execution on NVIDIA GPUs.
- An NVC++ command-line option, -stdpar, is used to enable GPU-accelerated C++ Parallel Algorithms

```
nvc++ -stdpar program.cpp -o program
```

RDF

Pseudo Code

```
for (int frame=0;frame<nconf;frame++) {
        for(int id1=0;id1<numatm;id1++) {
                for(int id2=0;id2<numatm;id2++) {
                        did1 = frame*numatm+id1
                        did2 = frame*numatm+id2
                        dx=d_x[did1]-d_x[did2];
                        dy=d_y[did1]-d_y[did2];
                        dz=d_z[did1]-d_z[did2];
                        r=sqrtf(dx*dx+dy*dy+dz*dz);

                        if (r<cut) {
                                ig2=(int)(r/del);
                                d_g2[ig2] = d_g2[ig2] +1 ;
                        }
                }
        }
}
```

- Across Frames
- Find Distance
- Reduction

STEPS

Step 1: Replace for with std::for_each

```
std::for_each (InputIterator first, InputIterator last, Function fn)

std::vector indices(numatm);
std::generate(indices.begin(), indices.end(), [n = 0]() mutable { return n++; });
```

start_iter : The beginning position from where function operations has to be executed.

last_iter : This ending position till where function has to be executed.

fnc/obj_fnc : The 3rd argument is a function or an object function which operation would be applied to each element.

STEPS

Step 2: Put function body inside Lambda

```
std::for_each(indices.begin(), indices.end(),
[...](unsigned int index)
                    {
                              for(int id2=0;id2<numatm;id2++)
                              {
                                        dx=d_x[]-d_x[];
                                        dy=d_y[]-d_y[];
                                        dz=d_z[]-d_z[];
                                        r=sqrtf(dx*dx+dy*dy+dz*dz);

                                        if (r<cut) {
                                                  ig2=(int)(r/del);
                                                  ++d_g2[ig2];
                                        }
                              }
                    }
          }
```

- Lambda : Convenient way of defining an anonymous function

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STEPS

Step 3: Pass execution policy as std::execution::par

```
for_each (std::execution::par , InputIterator first, InputIterator last, Function fn)
```

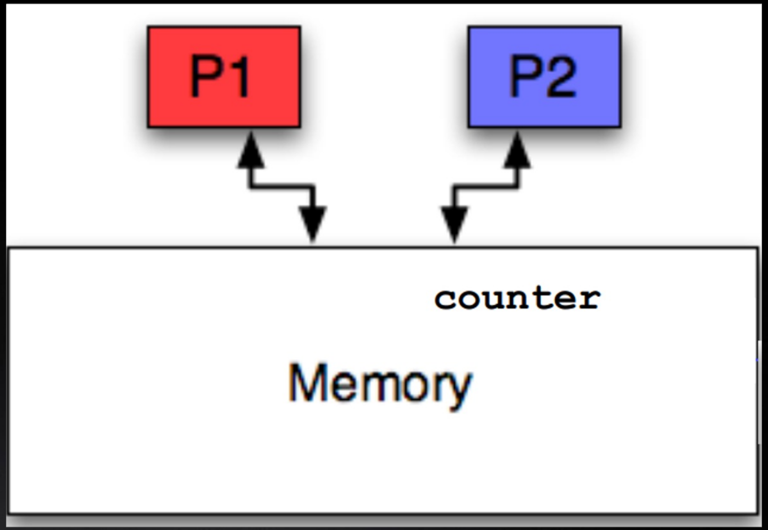
Execution policy as the first parameter will dictate to run the loop body in parallel across threads

ATOMIC

Step 4: Remove Datarace

```
std::atomic<int>* h_g2 = new std::atomic<int>[nbin];
```

```
void *do_stuff(void * arg)
{
        for (int i = 0 ; i < 200000000 ; ++ i)
        {  counter ++; }
        return arg;
}
```



Since the variable counter is shared, we can get a data race

STEPS

Step 5: Change indexing to use counting::iterator

```
std::for_each(std::execution::par,
                    thrust::counting_iterator<unsigned int>(0u),  thrust::counting_iterator<unsigned int>(numatm*)
```

```
std::vector<unsigned int> indices(numatm);
std::generate(indices.begin(), indices.end(), [n = 0]() mutable { return n++; });

std::for_each(std::execution::par,
          indices.begin(), indices.end(),
```

- Counting Iterator helps in filling up a vector with the numbers zero through N
- In our case from 0 to number of atoms
- GPU We will be using Thrust library for counting iterator for GPU
  - High-Level Parallel Algorithms Library
  - Parallel Analog of the C++ Standard Template Library (STL)

STEPS

Step 5: Compile for Multicore and GPU

```
std::atomic<int>* h_g2 = new std::atomic<int>[nbin];

std::for_each(std::execution::par, thrust::counting_iterator<unsigned int>(0u),
                                   thrust::counting_iterator<unsigned int>(numatm),
          [...](unsigned int index)
                {
                          for(int id2=0;id2<numatm;id2++)
                          {
                                    dx=d_x[]-d_x[];
                                    dy=d_y[]-d_y[];
                                    dz=d_z[]-d_z[];
                                    r=sqrtf(dx*dx+dy*dy+dz*dz);

                                    if (r<cut) {
                                              ig2=(int)(r/del);
                                              ++d_g2[ig2];
                                    }
                          }
                }
          }
```

- Atomic Declaration
- Counting Iterator
- Find Distance
- Atomic Increment

```
nvc++ -stdpar=gpu,multicore program.cpp -o program
```

WORKSHOP

Modify rdf.cpp / rdf.f90

1. Index maps to id1 / id2

```
for(int index = 0; index < numatm*numatm; index++) {
    id1=index/numatm;
    id2=index%numatm;
    …;
}
```

2. for_each and std::execution::par(multicore) / std::execution::par_unseq(GPU)

3. counting iterator

FORTRAN

DO CONCURRENT :: ISO Standard Fortran

- ISO Standard Fortran 2008 introduced the DO CONCURRENT construct to allow you to express loop-level parallelism, one of the various mechanisms for expressing parallelism directly in the Fortran language
- HPC SDK 20.11 release of the NVIDIA HPC SDK, the included NVFORTRAN compiler automatically accelerates DO CONCURRENT

```
subroutine saxpy(x,y,n,a)
  real :: a, x(:), y(:)
  integer :: n, i
  do i = 1, n
    y(i) = a*x(i)+y(i)
  enddo
end subroutine saxpy
```

```
subroutine saxpy(x,y,n,a)
  real :: a, x(:), y(:)
  integer :: n, i
  do concurrent (i = 1: n)
    y(i) = a*x(i)+y(i)
  enddo
end subroutine saxp
```

```
nvfortran –stdpar=gpu,multicore program.f90 -o program
```

FORTRAN

Nested Loop Parallelism

- Nested loops are a common code pattern encountered in HPC applications
- It is straightforward to write such patterns with a single DO CONCURRENT statement, as in the following example

```
do i=2, n-1
  do j=2, m-1
    a(i,j) = w0 * b(i,j)
  enddo
enddo
```

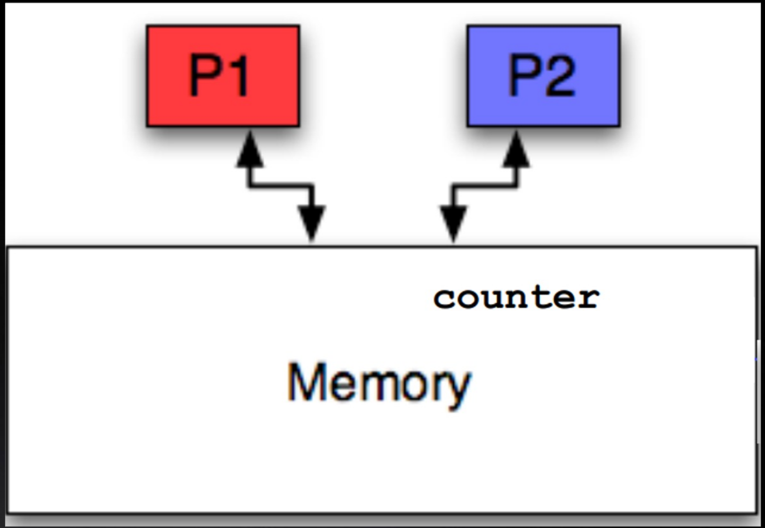
```
do concurrent(i=2 : n-1, j=2 : m-1)
  a(i,j) = w0 * b(i,j)
enddo
```

ATOMIC

Limitation

```
!$acc atomic
g(ind)=g(ind)+1.0d0
```

```
void *do_stuff(void * arg)
{
        for (int i = 0 ; i < 200000000 ; ++ i)
        {  counter ++; }
        return arg;
}
```



- Do-Concurrent implementation of GPC SDK currently does not support Atomic constructs
- Hence we use the OpenACC Construct to solve data race

STEPS

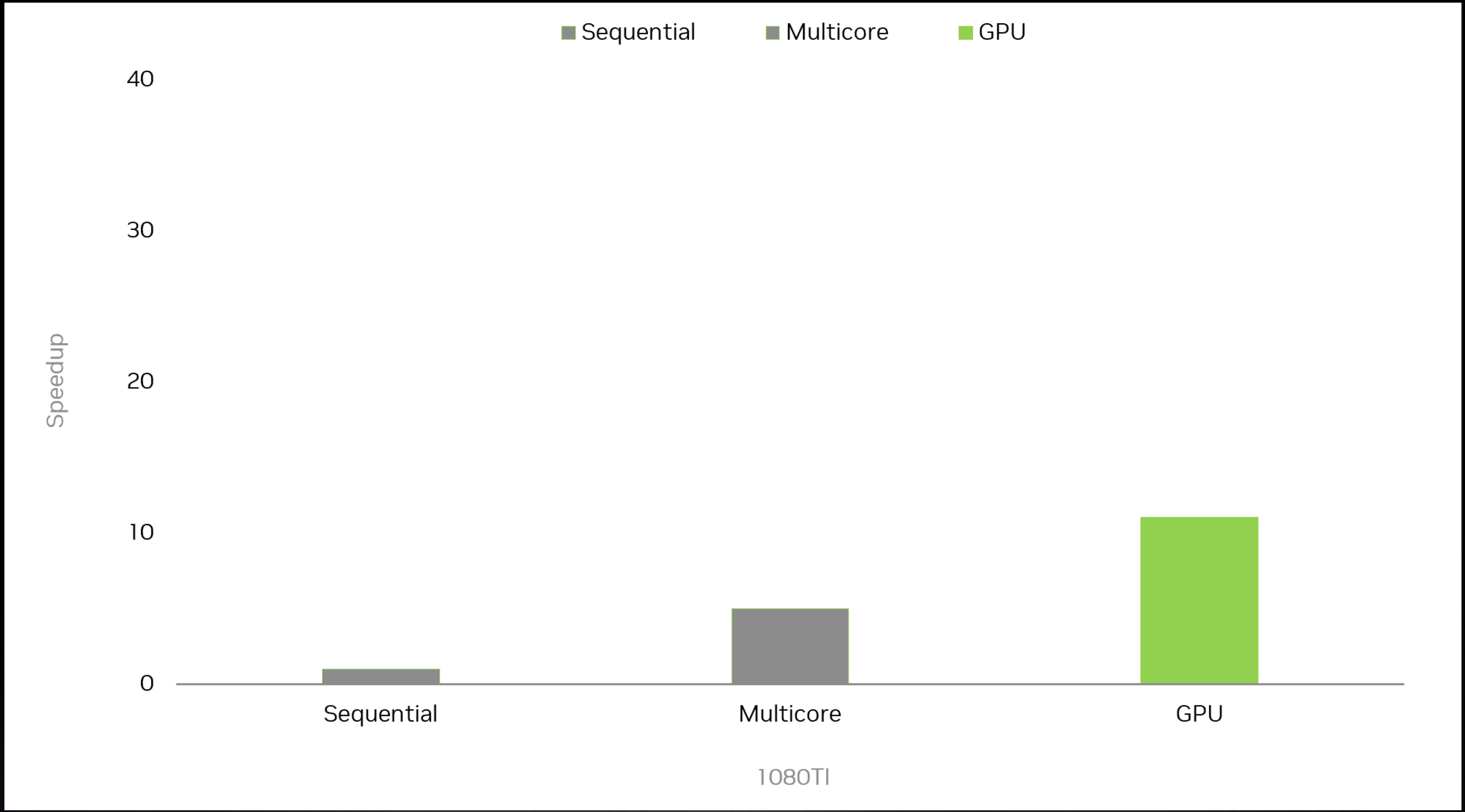
Compile for Multicore and GPU

```
do iconf=1,nframes

      do concurrent(i=1 : natoms, j=1:natoms)
          dx=x(iconf,i)-x(iconf,j)
          dy=y(iconf,i)-y(iconf,j)
          dz=z(iconf,i)-z(iconf,j)

                      …
          r=dsqrt(dx**2+dy**2+dz**2)
               if(r<cut)then
            !$acc atomic
                         g(ind)=g(ind)+1.0d0
          endif
      enddo
    enddo
```

- Do Concurrent
- Find Distance
- Atomic Increment

```
nvfortran -stdpar=gpu,multicore program.f90 -o program
```

STD::PAR SPEEDUP



HPC SDK 20.11, NVIDIA GTX1080TI

KNOWN LIMITATIONS

LIMITATIONS

Heap Only

- Limitation: All pointers used in parallel algorithms must point to the heap

```
std::array<int, 1024> a = ...;

std::sort(std::execution::par, a.begin(), a.end()); // Fails, array stored on the stack
```

- Solution: Use function objects or lambdas instead

```
std::vector v = new ; std::sort(std::execution::par, v.begin(), v.end()); // OK, vector allocates on heap
```

LIMITATIONS

FUNCTION POINTERS

- Limitation: Don’t pass function pointers to algorithms that will run on the GPU

```
void square(int& x) { x = x * x; }

std::for_each(std::execution::par, v.begin(), v.end(),  &square); // Fails: uses raw function pointer
```

- Solution: Use function objects or lambdas instead

```
struct square {
        void operator()(int& x) const { x = x * x; }
};

std::for_each(std::execution::par, v.begin(), v.end(), square()); // OK, function object

std::for_each(std::execution::par, v.begin(), v.end(), [](int& x) { x = x * x; }); // OK, lambda
```

OTHER LIMITATIONS

- GPU code does not have access to the operating system or pre-compiled standard library
- Usually works:
  - template classes and functions
  - inlined functions
  - math functions
- Usually doesn't work:
  - non-template library functions
  - OS functions

WE WILL BE BACK AT 11: 00

REFERENCES

https://developer.nvidia.com/blog/accelerating-fortran-do-concurrent-with-gpus-and-the-nvidia-hpc-sdk/

https://developer.nvidia.com/blog/accelerating-standard-c-with-gpus-using-stdpar/

https://developer.download.nvidia.com/video/gputechconf/gtc/2019/presentation/s9770-c++17-parallel-algorithms-for-nvidia-gpus-with-pgi-c++.pdf

THANK YOU

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