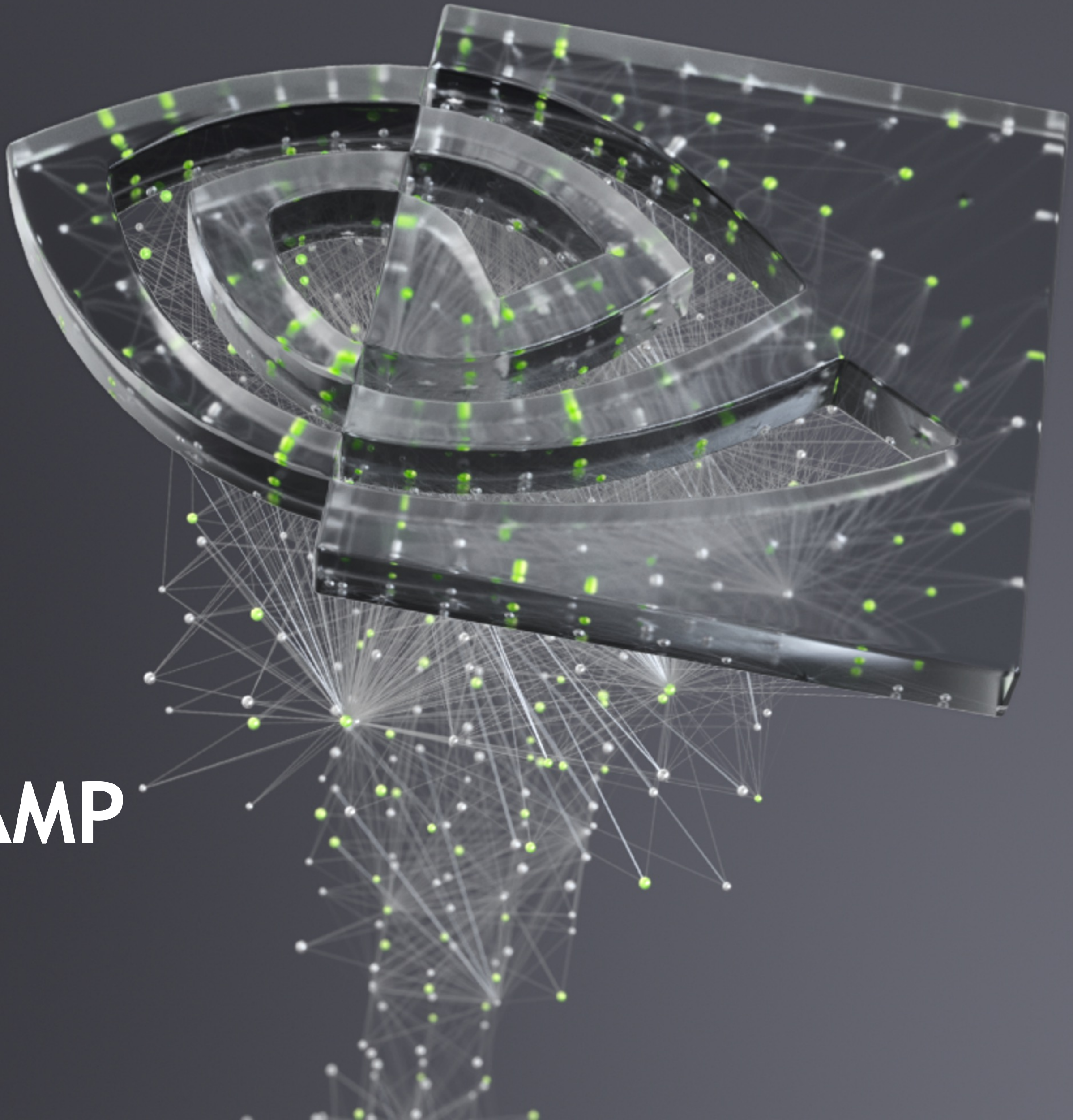

N-WAYS GPU BOOTCAMP

STANDARD LANGUAGES

STANDARD LANGUAGES

What to expect?

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

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BRIEF HISTORY

- Historically, accelerating your code with GPUs has not been possible in Standard C++/Fortran without using language extensions or additional libraries:
  - CUDA C++ requires the use of `__host__` and `__device__` attributes on functions and the `<<<>>>` syntax for GPU kernel launches.
  - OpenACC uses `#pragmas` to control GPU acceleration

- What if you could take your Standard C++ or Fortran code and accelerate on a GPU?

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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

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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.

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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
```

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RDF

Pseudo Code

```
for (int frame=0;frame<nconf;frame++){

  for(int id1=0;id1<numatm;id1++)
  {
    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] = d_g2[ig2] +1 ;
      }
    }
  }
}
```

- Across Frames
- Find Distance
- Reduction

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STEPS

Step 1: Replace for with std::for_each

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

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.

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STEPS

Step 2: 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

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STEPS

Step 3: Change indexing to use counting::iterator

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

```
std::vector<unsigned int> indices(numatm * 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)

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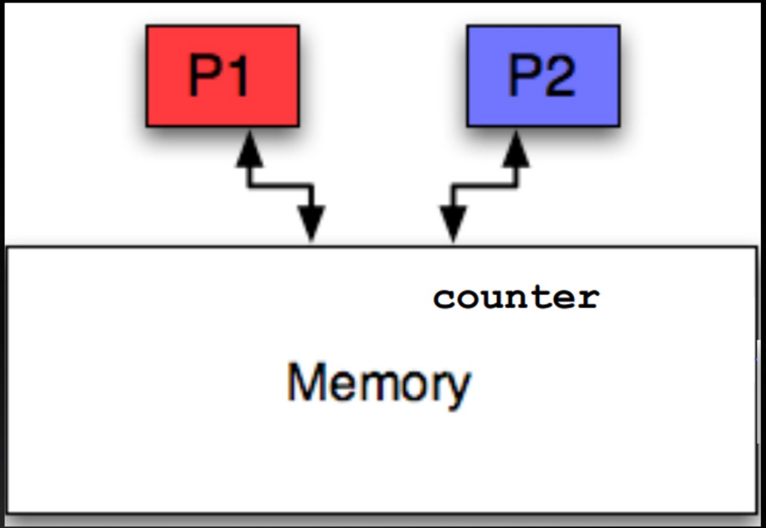
ATOMIC

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

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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*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
```

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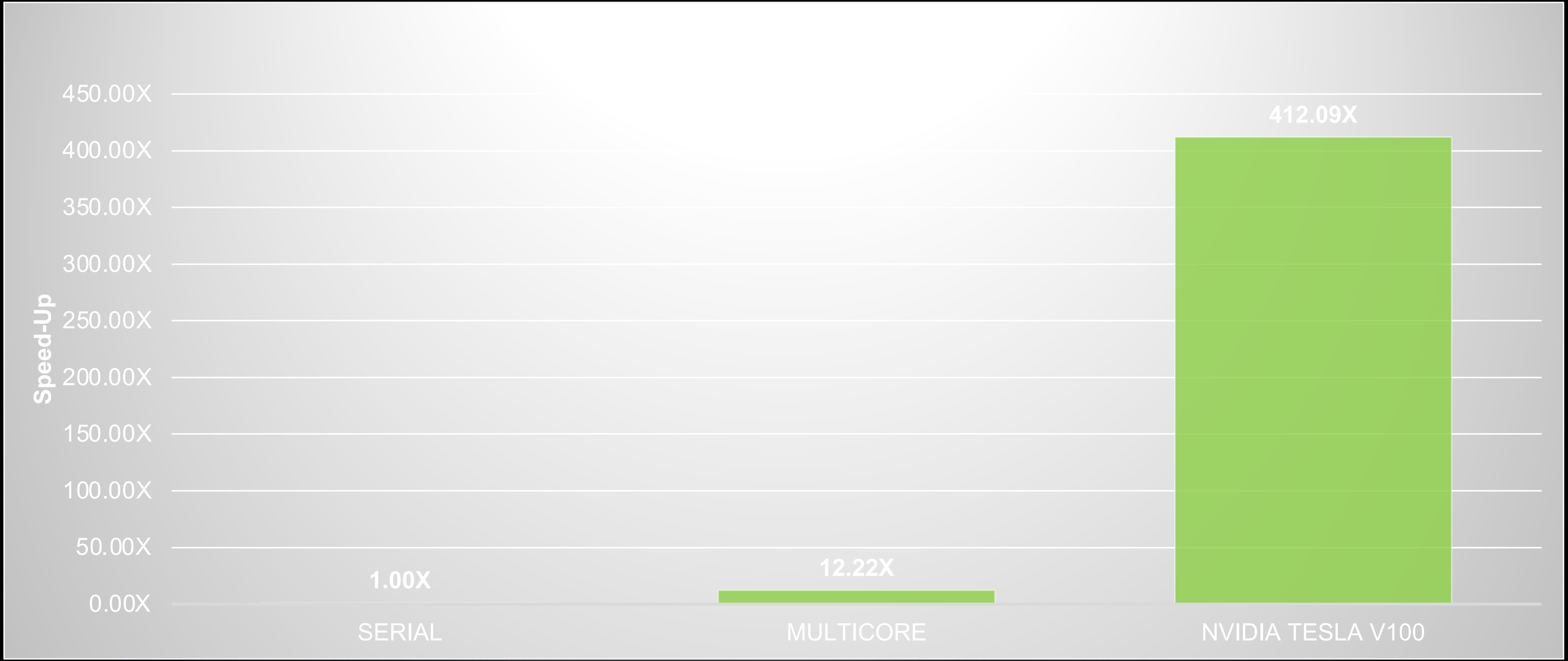
STD::PAR SPEEDUP



HPC SDK 20.11, NVIDIA Tesla V100, DGX1

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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
```

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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
```

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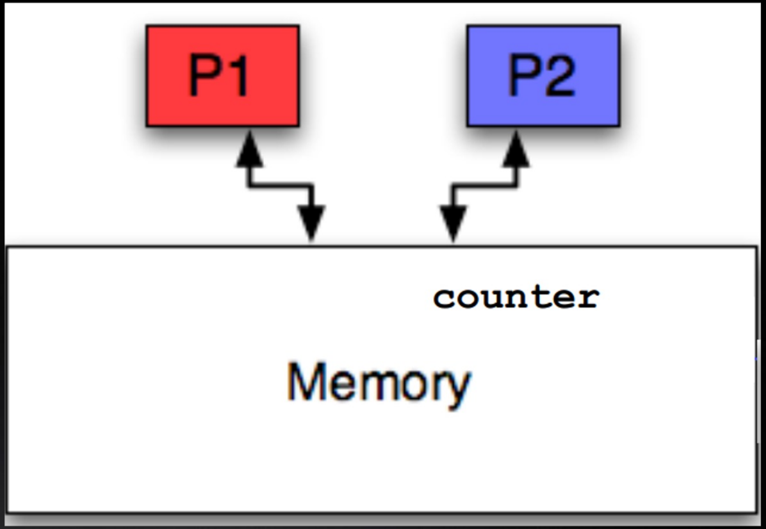
ATOMIC

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

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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
```

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WE WILL BE BACK AT 13: 00

REFERENCES

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

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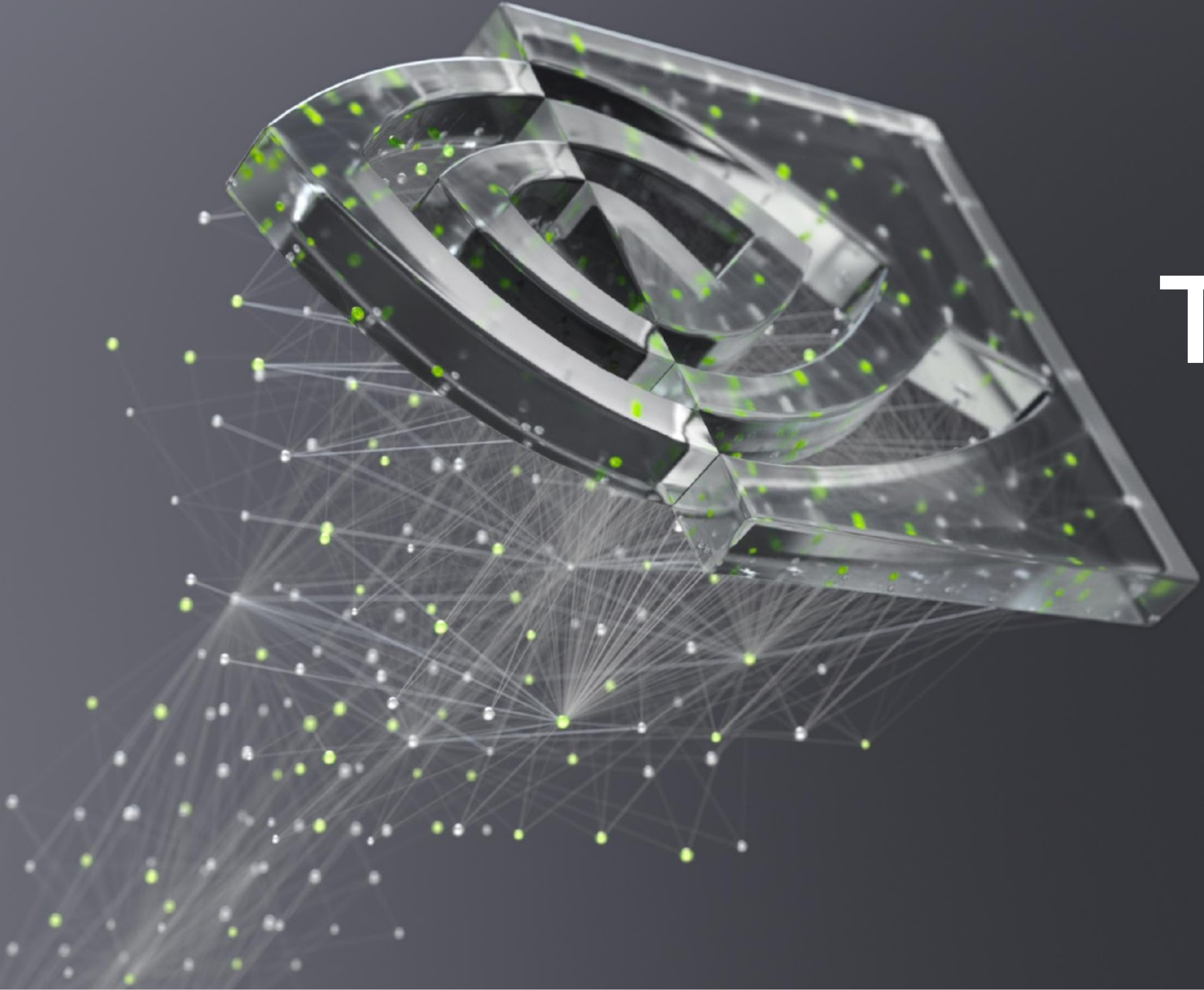

THANK YOU