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CUDA Runtime API & Core Libraries

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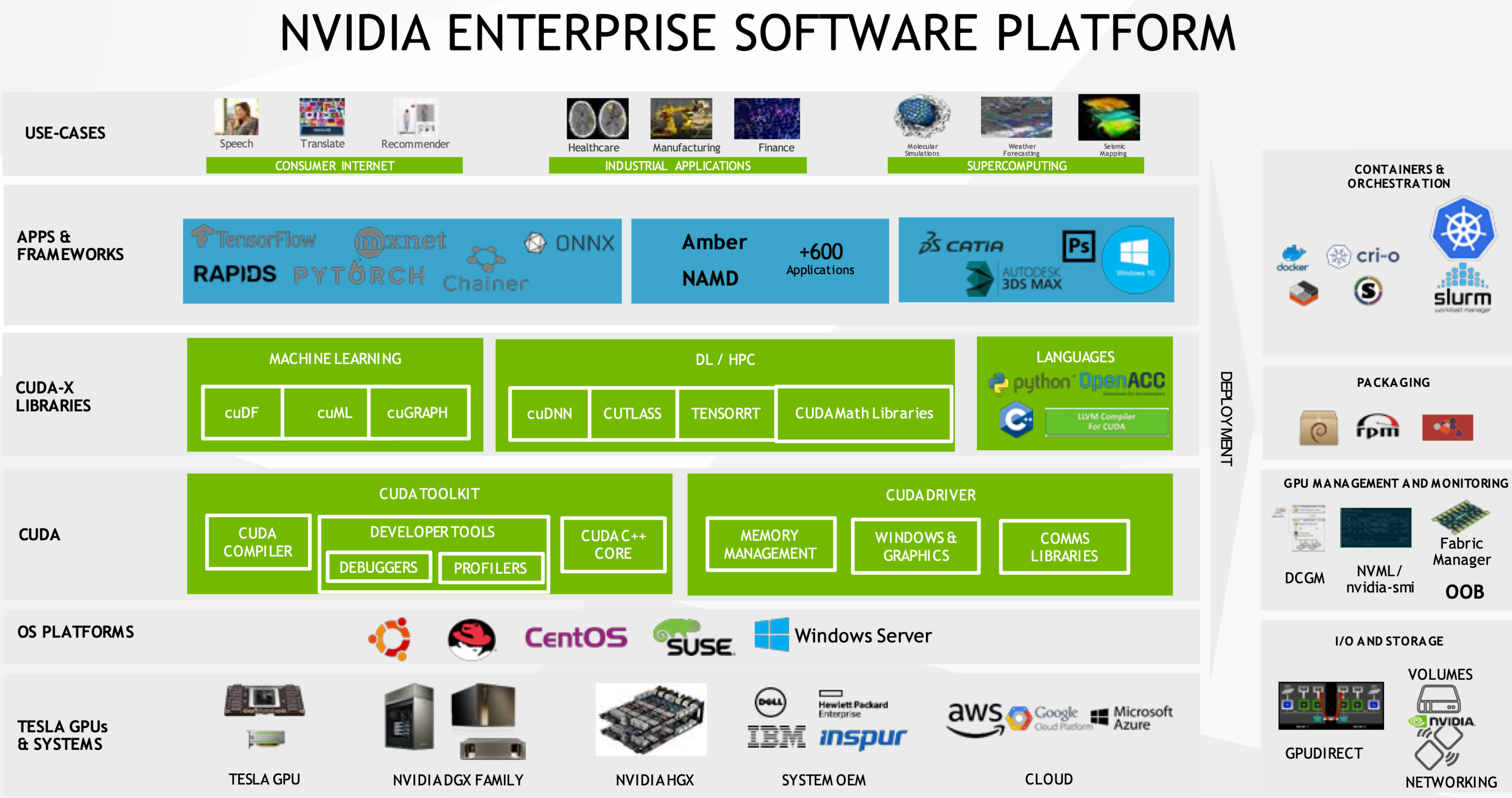
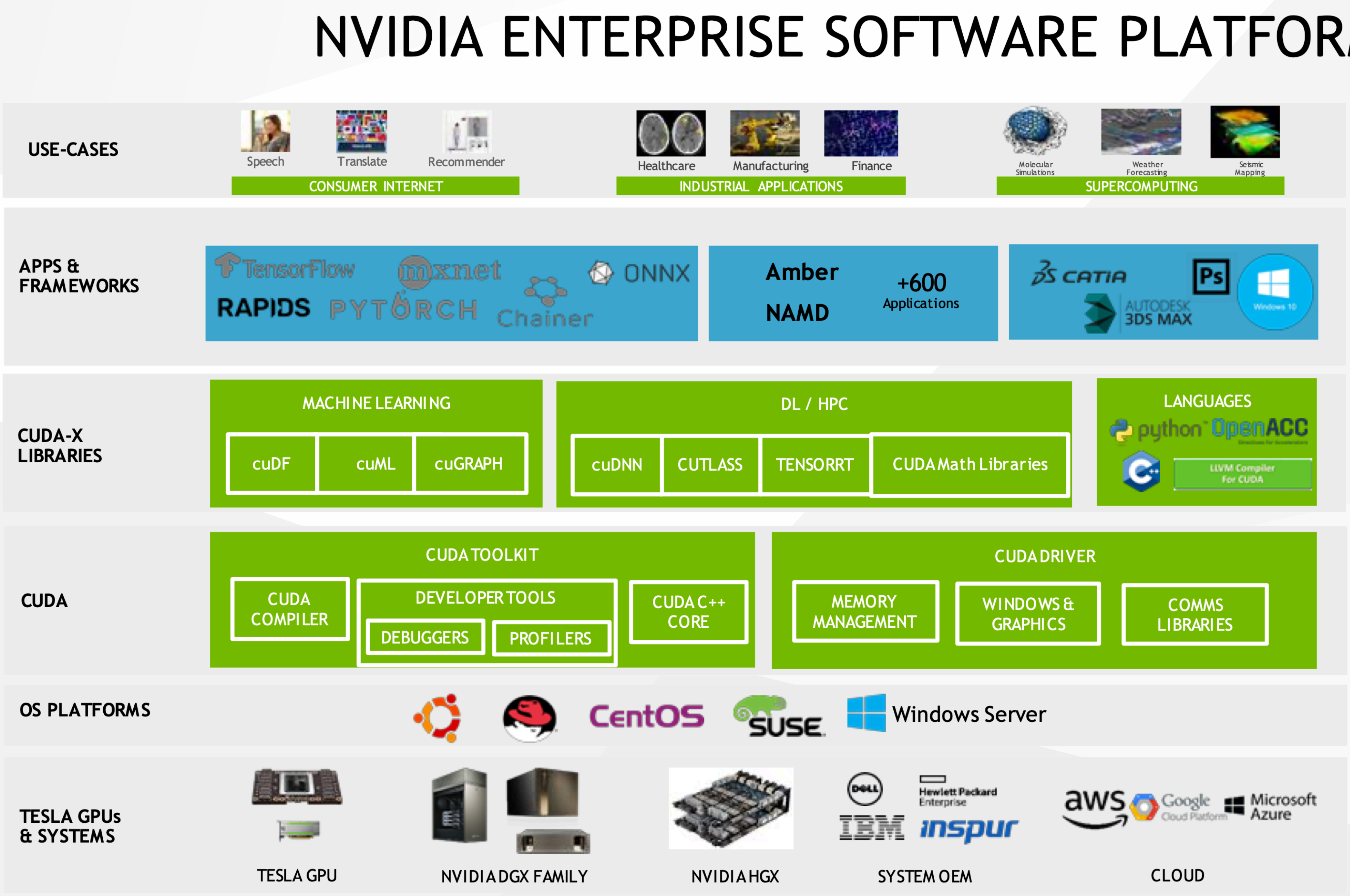
CUDA Software Ecosystem



CUDA Software Ecosystem

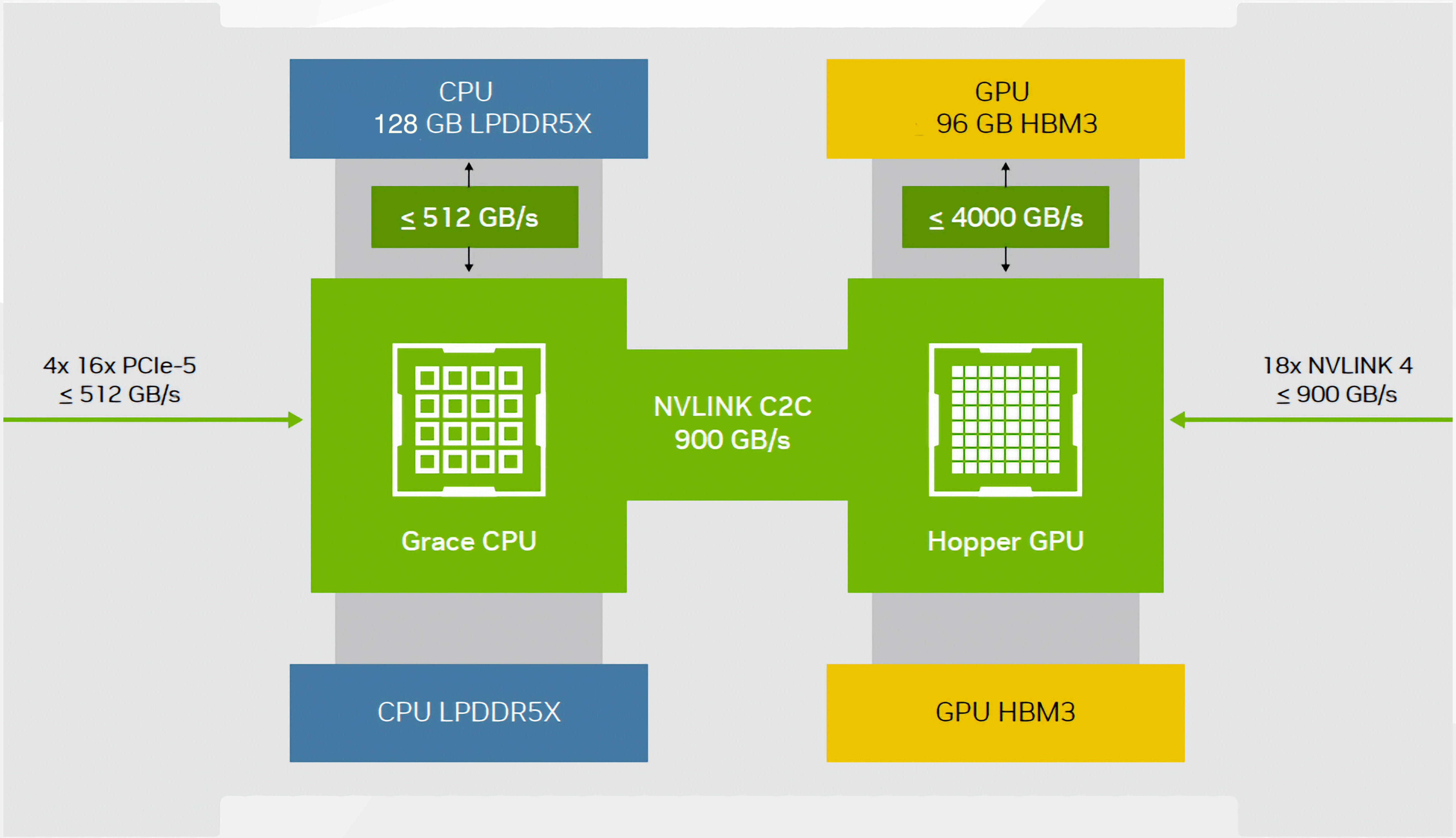


No GPU details visible to user

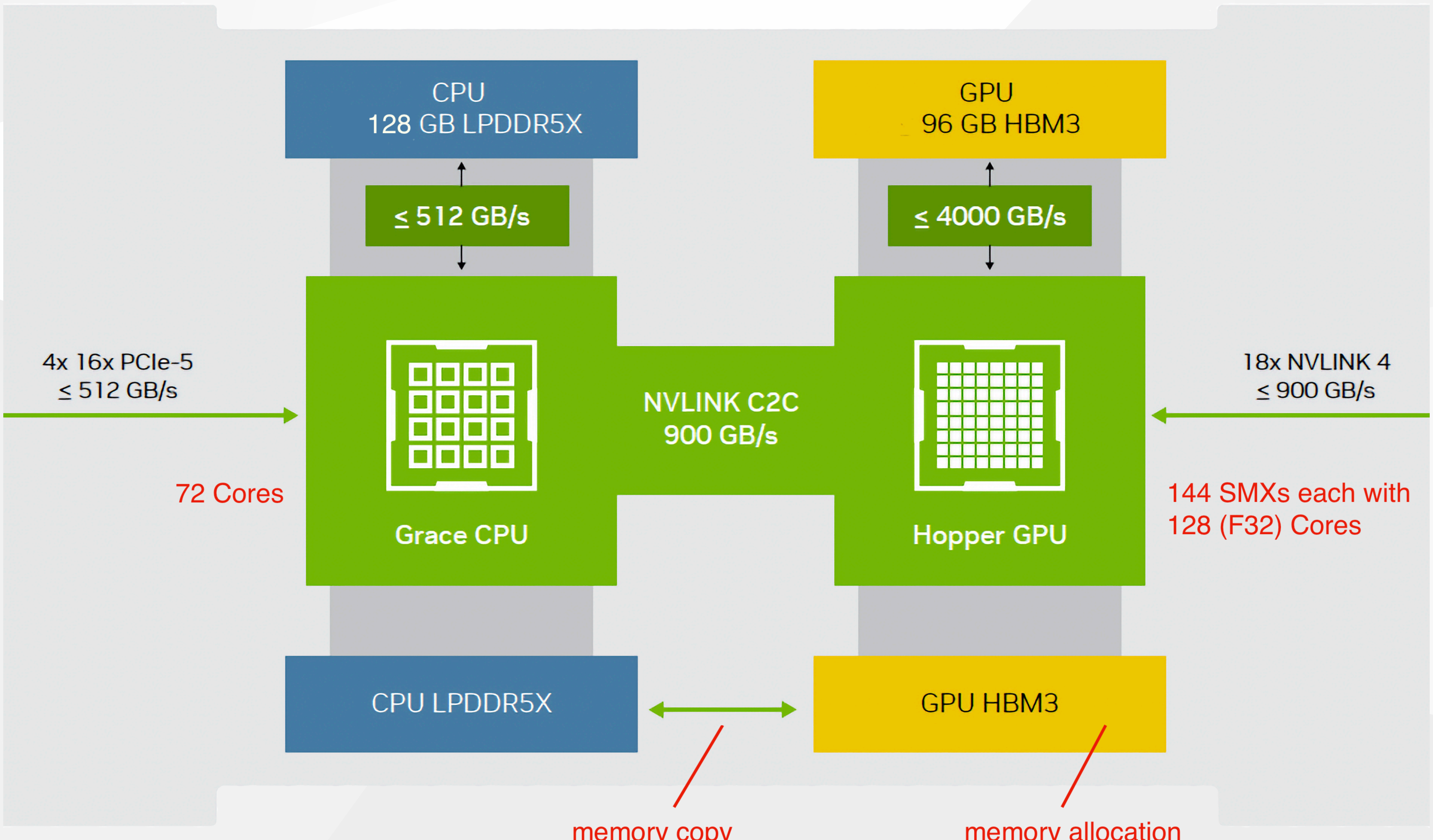
No GPU kernel code, but user manages GPU memory

Development of GPU kernel code

Hardware & Memory on a Daint Node



Hardware & Memory on a Daint Node



Host & Device Memory Spaces

- The GPU has separate memory to the host CPU
  - The host CPU has 128 GB of DDR5 **host memory**
  - The H100 GPU has 96 GB of HBM3 **device memory**
- Kernels executing on the GPU have fast access to device memory, and much slower access to host memory
  - Kernel accesses to host memory are copied to GPU memory first over the (slower) NVLINK connections (PCI-e for older/consumer hardware)

hardware	bandwidth	remarks
host $\leftrightarrow$ device	450×2 GB/s	NVLINK
host memory	512 GB/s	LPDDR5X
device memory	4000 GB/s	HBM3

- **Optimization Tip**: The massive bandwidth of HBM3 on H100 GPUs can only help if data is in the right memory space **before** the computation starts

CUDA Runtime API

- Is a **host** library for orchestrating interactions with the device
  - allocate memory on the device
  - copy data between host and device
  - launch device functions, i.e. kernels
- API functions start with `cuda...`
  - `cudaMalloc`
  - `cudaMemcpy`
  - `<<<...>>>` kernel launch
- Calls are made from **CPU** code

Allocating Device Memory with `cudaMalloc`

- Can’t be read from host
  - host has the pointer to device memory
  - but the host cannot de-reference the pointer
- Need to manually copy data to and from host
- For memory that should always reside on device

Allocating Device Memory

`cudaMalloc(void** ptr, size_t size)`

- `size` number of **bytes** to allocate
- `ptr` points to allocated memory on return

Freeing Device Memory

`cudaFree(void* ptr)`

Allocate Memory for 100 doubles on Device

```
double* v; // C pointer that will point to device memory
auto bytes = 100*sizeof(double); // size in bytes!
cudaMalloc(&v, bytes); // allocate memory
cudaFree(v);           // free memory
```

Copying Memory with `cudaMemcpy`

- Accepts device pointers obtained with `cudaMalloc`
- Uses the NVLINK (on PCI-Express on older GPUs) to copy between the host and device
- Can also be used for copies within the device

Perform Blocking Copy

This is when host waits for copy to finish before executing any other task.

```
cudaMemcpy(void *dst, void *src, size_t size, cudaMemcpyKind kind)
```

- `dst` destination pointer
- `src` source pointer
- `size` number of **bytes** to copy to `dst`
- `kind` enumerated type specifying direction of copy:
  one of `cudaMemcpyHostToDevice`, `cudaMemcpyDeviceToHost`,
  `cudaMemcpyDeviceToDevice` or `cudaMemcpyHostToHost`

Copy 100 doubles to Device, then back to Host

```
auto size = 100*sizeof(double);       // size in bytes
double *v_d;
cudaMalloc(&v_d, size);               // allocate on device
double *v_h = (double*)malloc(size); // allocate on host
cudaMemcpy(v_d, v_h, size, cudaMemcpyHostToDevice);
cudaMemcpy(v_h, v_d, size, cudaMemcpyDeviceToHost);
```

Errors Handling

- All API functions return error codes that indicate either:
    - success;
    - an error in the API call;
    - an error in an earlier asynchronous call.
- The return value is the enum type `cudaError_t`. e.g.

```
cudaError_t status = cudaMalloc(&v, 100);
```

- status is { `cudaSuccess` , `cudaErrorMemoryAllocation` }
- The following returns a string describing status

```
const char* cudaGetErrorString(status)
```

- `cudaError_t cudaGetLastError()` returns the last error
- resets status to `cudaSuccess`

Copy 100 doubles to Device, then back to Host with error checking

```
double *v_d;
auto size = sizeof(double)*100;
double *v_host = (double*)malloc(size);
cudaError_t status;

status = cudaMalloc(&v_d, size);
if(status != cudaSuccess) {
  printf("cuda error : %s\n", cudaGetErrorString(status));
  exit(1);
}

status = cudaMemcpy(v_d, v_h, size, cudaMemcpyHostToDevice);
if(status != cudaSuccess) {
  printf("cuda error : %s\n", cudaGetErrorString(status));
  exit(1);
}
```

It is essential to test for errors

But it is tedious and obfuscates our source code if it is done in line for every API and kernel call. . .

Exercise: Device Memory API

Open `cuda/practicals/api/util.hpp`

1. what does `cuda_check_status()` do?
2. look at the template wrappers `malloc_host` & `malloc_device`
   - what do they do?
   - what are the benefits over using `malloc` and `cudaMalloc` directly?
   - do we need corresponding functions for `cudaFree` and `free` ?
3. write a wrapper around `cudaMemcpy` for copying data host→device & device→host
   - remember to check for errors!
4. compile the test and run
   it will pass with no errors on success

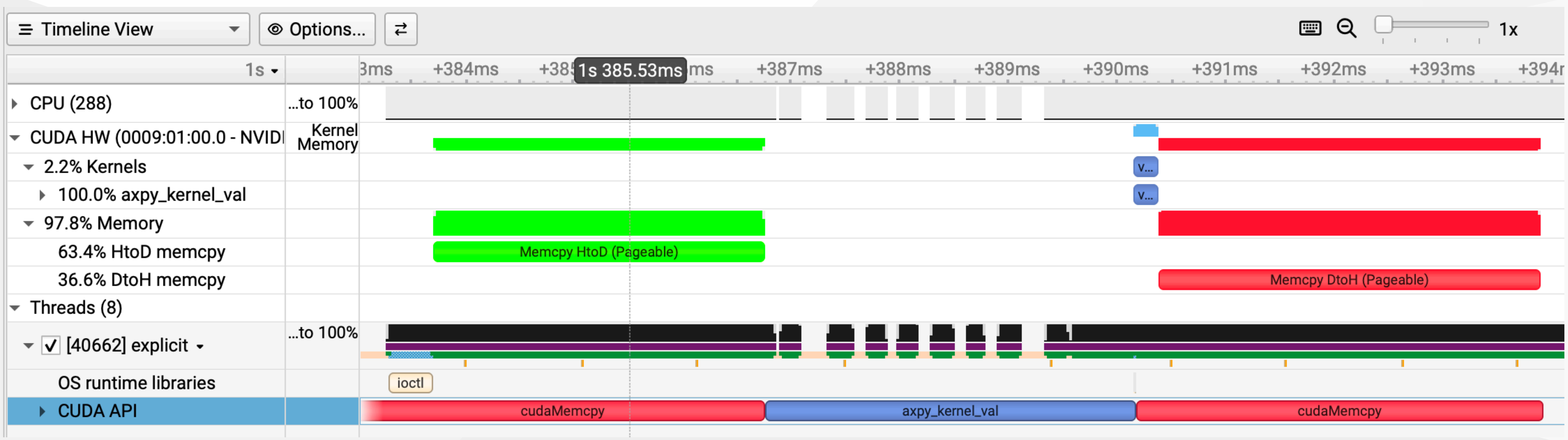
```
> make explicit
> srun ./explicit 8
```

Demo: Profiling with NVIDIA Nsight Systems

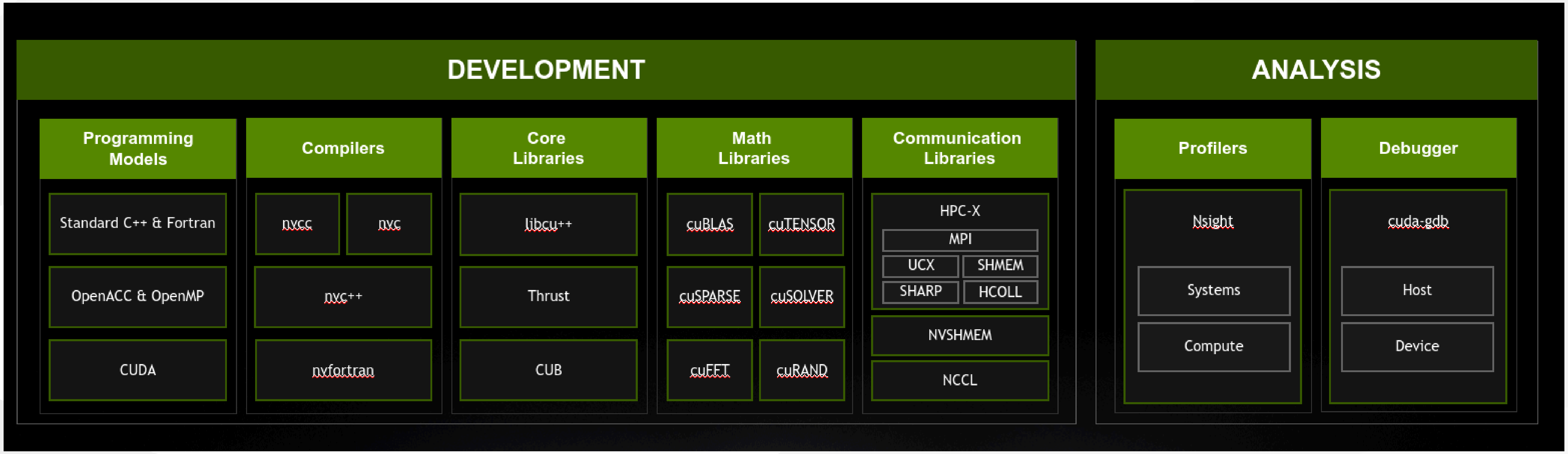
Run `nsys` profiler on daint and generate a report

```
> srun nsys profile ./explicit 25
```

Download the report and open it locally in Nsight Systems



Using CUDA Libraries



Managing GPU memory with allocations and data transfers is already enough to call various GPU libraries, such as:

- sorting, reductions, prefix sums
- linear algebra and solvers
- FFT
- etc...

Remarks about `cuBLAS`

Excerpt from the `cuBLAS` Example

```
#include <cublas_v2.h>

cublasHandle_t cublas_handle;
cublasCreate(&cublas_handle);

auto cublas_status = cublasDaxpy(cublas_handle, n, &alpha, x_device, 1, y_device, 1);
```

- Implements BLAS operations for the device
- Compiled library: need an include file and link against `-lcublas`
- Expects device pointers (from `cudaMalloc`)
- Data transfer to/from the device is the user's responsiblity
- Launched on the host (device-launched version is a separate library)

Core libraries: CUB and Thrust

- CUB (Cuda UnBound) and Thrust are header-only
- requires `nvcc` to compile kernel code
- **CUB**
  - is CUDA specific
  - contains header functions for use in device kernel code
  - contains higher-level operations to launch from host
- **Thrust**
  - is platform agnostic
  - implements algorithms of the C++ STL CUDA backend - built on top of CUB launched from host
- both are built on top of and inter-operable with the CUDA runtime API

Some Thrust Examples

host and device vectors

```
#include <thrust/host_vector.h>
#include <thrust/device_vector.h>

thrust::device_vector<double> d_vector;
thrust::host_vector<double>   h_vector(10);

// performs cudaMalloc and cudaMempcpy host->device
d_vector = h_vector;

// performs cudaMempcpy device->host
h_vector = d_vector;
```

sorting

```
#include <thrust/sort.h>

thrust::sort(thrust::device, d_vector.begin(), d_vector.end());
```

reductions

```
#include <thrust/reduce.h>

thrust::reduce(thrust::device, d_vector.begin(), d_vector.end(), 0);
```

Using Thrust with the Runtime API

thrust sort with C-pointers

```
#include <thrust/device_vector.h>
#include <thrust/sort.h>

double* d_v;
cudaMalloc(&d_v, 100*sizeof(double));

thrust::sort(thrust::device,
             thrust::device_pointer_cast(d_v),
             thrust::device_pointer_cast(d_v + 100));
```

Exercise: Sorting with Thrust

1. How does the performance of `std::sort` on the host compare against `thrust::sort` on the device?
2. What if the data transfer times to and from device are included?