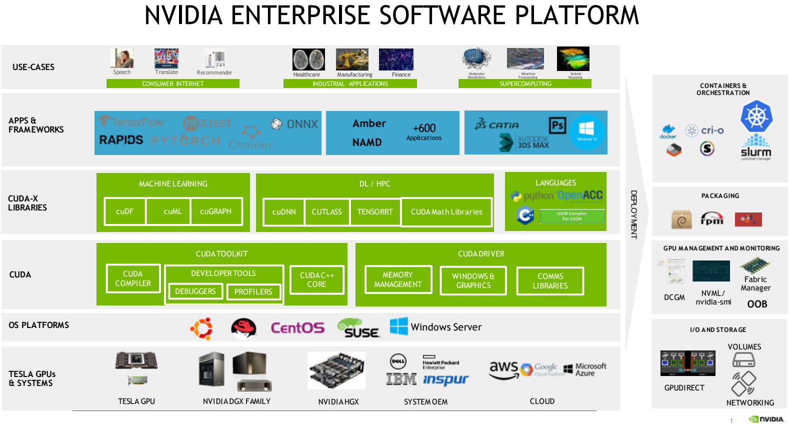
CSCS
Centro Svizzero di Calcolo Scientifico
Swiss National Supercomputing Centre

ETH zürich

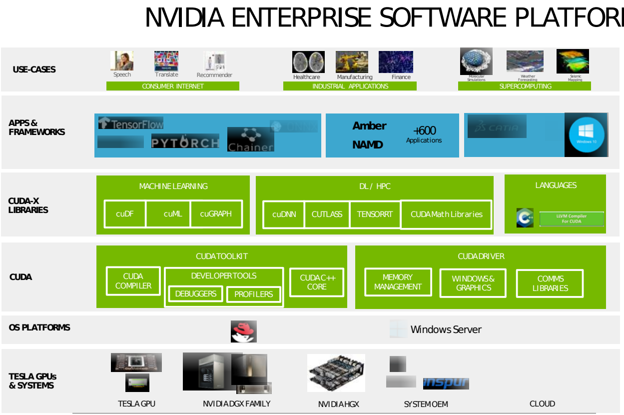
CUDA runtime API and core libraries

Sebastian Keller, Prashanth Kanduri and Ben Cumming, CSCS

The software ecosystem on top of CUDA



The software ecosystem on top of CUDA

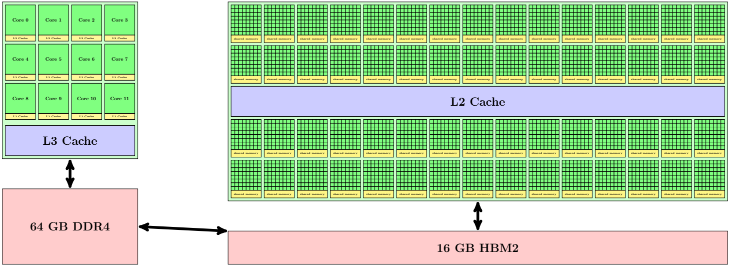


GPU details invisible to user

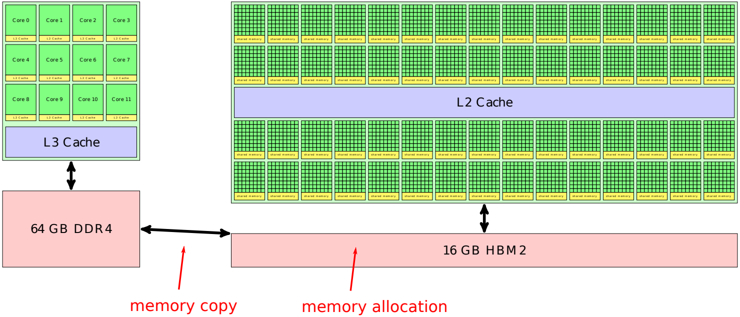
No GPU kernel code, but user manages GPU memory

Development of GPU kernel code

Hardware and memory on a Piz Daint Node



Hardware and memory on a Piz Daint Node



Host and Device Memory Spaces

- The GPU has separate memory to the host CPU
  - The host CPU has 64 GB of DDR4 **host memory**
  - The P100 GPU has 16 GB of HBM2 **device memory**
- Kernels executing on the GPU only have fast access to device memory
  - Kernel accesses to host memory are copied to GPU memory first over the (slow) PCIe connection.

host $\leftrightarrow$ device	11×2 GB/s	PCIe gen3
host memory	45 GB/s	DDR4
device memory	558 GB/s	HBM2

- **Optimization tip**: The massive bandwidth of HBM2 on P100 GPUs can only help if data is in the right memory space **before** computation starts.

The 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 PCI-Express bus to copy between the host and device
- Can also be used for copies within the device

Perform blocking copy (host waits for copy to finish)

```
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`, `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 happen...

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`}

Handling errors

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

- returns a string describing status

```
cudaError_t cudaGetLastError()
```

- returns the last error
- resets status to `cudaSuccess`

Copy 100 doubles to device **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 `topics/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 `cudaMalloc` and `free` 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
```

Exercise: Device Memory API

What does the nvprof profile look like?

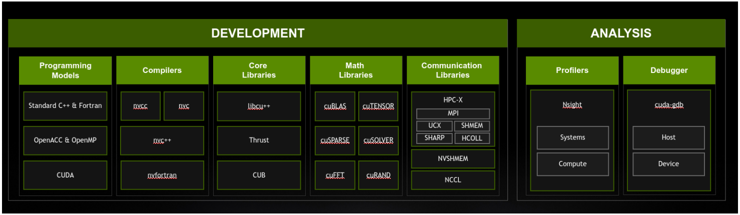
```
> srun nvprof -o explicit.nvvp --profile-from-start off -f
    ./explicit 25
> nvvp explicit.nvvp &
```

Note about `nvprof`

For devices newer than the P100, the functionality of `nvprof` is now offered in two new tools:

- `nsight-sys`
- `nsight-compute`.

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...

Some 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 inlude 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)
    ;
```

Thrust interoperability 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?