CSCS
Centro Svizzero di Calcolo Scientifico
Swiss National Supercomputing Centre

ETH zürich

CUDA Runtime API & Core Libraries

CSCS Summer School 2023

Sebastian Keller, Prashanth Kanduri, Jonathan Coles & Ben Cumming

CUDA Software Ecosystem

NVIDIA ENTERPRISE SOFTWARE PLATFORM

USE-CASES

Speech | Translate | Recommender — CONSUMER INTERNET

Healthcare | Manufacturing | Finance — INDUSTRIAL APPLICATIONS

Molecular Simulations | Weather Forecasting | Seismic Mapping — SUPERCOMPUTING

APPS & FRAMEWORKS

TensorFlow, mxnet, ONNX, RAPIDS, PYTORCH, Chainer

Amber, NAMD, +600 Applications

CATIA, Ps, AUTODESK 3DS MAX, Windows 10

CUDA-X LIBRARIES

MACHINE LEARNING: cuDF | cuML | cuGRAPH

DL / HPC: cuDNN | CUTLASS | TENSORRT | CUDA Math Libraries

LANGUAGES: python | OpenACC | C++ | LLVM Compiler For CUDA

CUDA

CUDA TOOLKIT: CUDA COMPILER | DEVELOPER TOOLS (DEBUGGERS | PROFILERS) | CUDA C++ CORE

CUDA DRIVER: MEMORY MANAGEMENT | WINDOWS & GRAPHICS | COMMS LIBRARIES

OS PLATFORMS

CentOS | SUSE | Windows Server

TESLA GPUs & SYSTEMS

TESLA GPU | NVIDIA DGX FAMILY | NVIDIA HGX | SYSTEM OEM (DELL, Hewlett Packard Enterprise, IBM, inspur) | CLOUD (aws, Google Cloud Platform, Microsoft Azure)

DEPLOYMENT

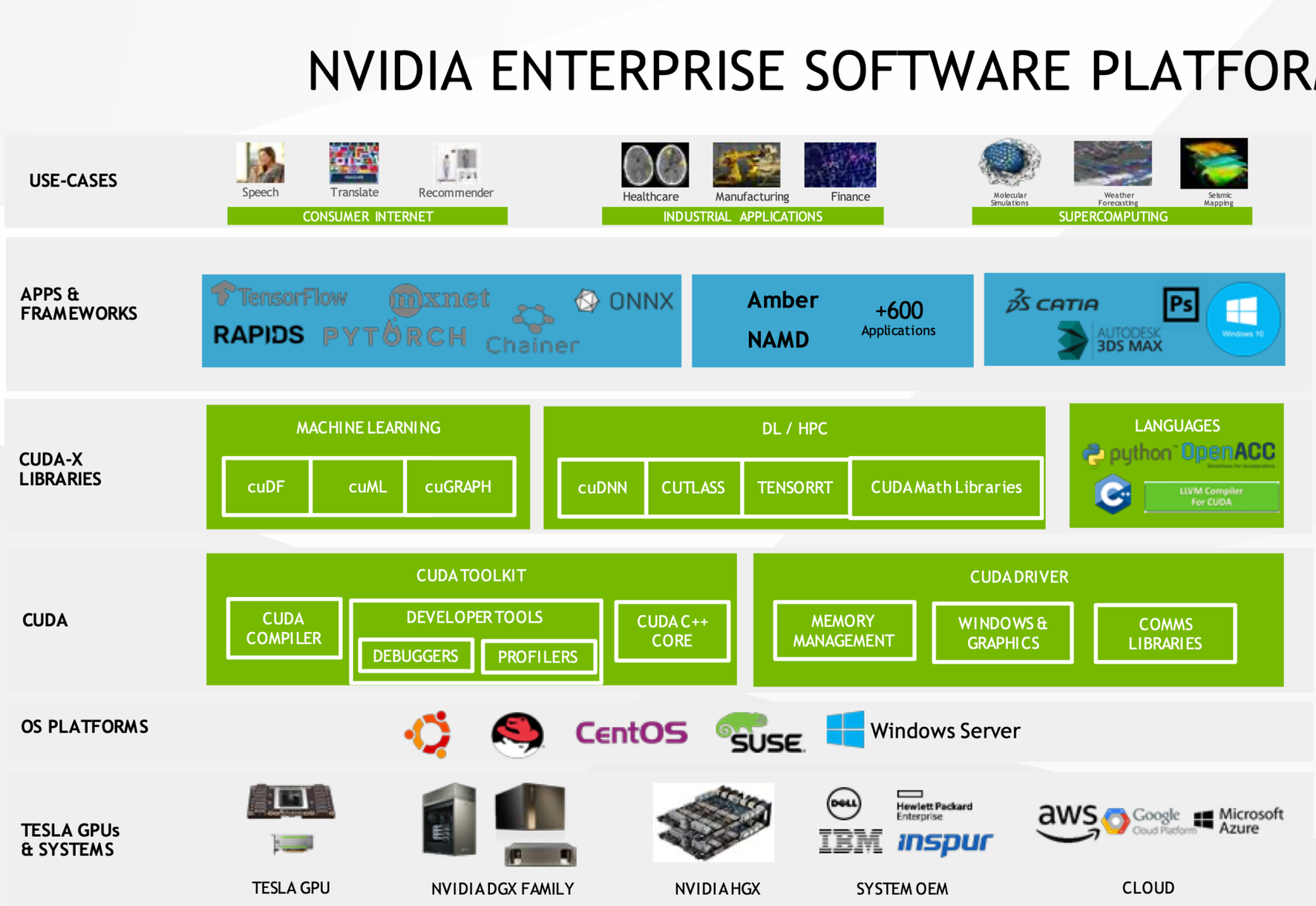
CONTAINERS & ORCHESTRATION: docker | cri-o | slurm

PACKAGING

GPU MANAGEMENT AND MONITORING: DCGM | NVML / nvidia-smi | Fabric Manager | OOB

I/O AND STORAGE: GPUDIRECT | VOLUMES | NETWORKING

CUDA Software Ecosystem

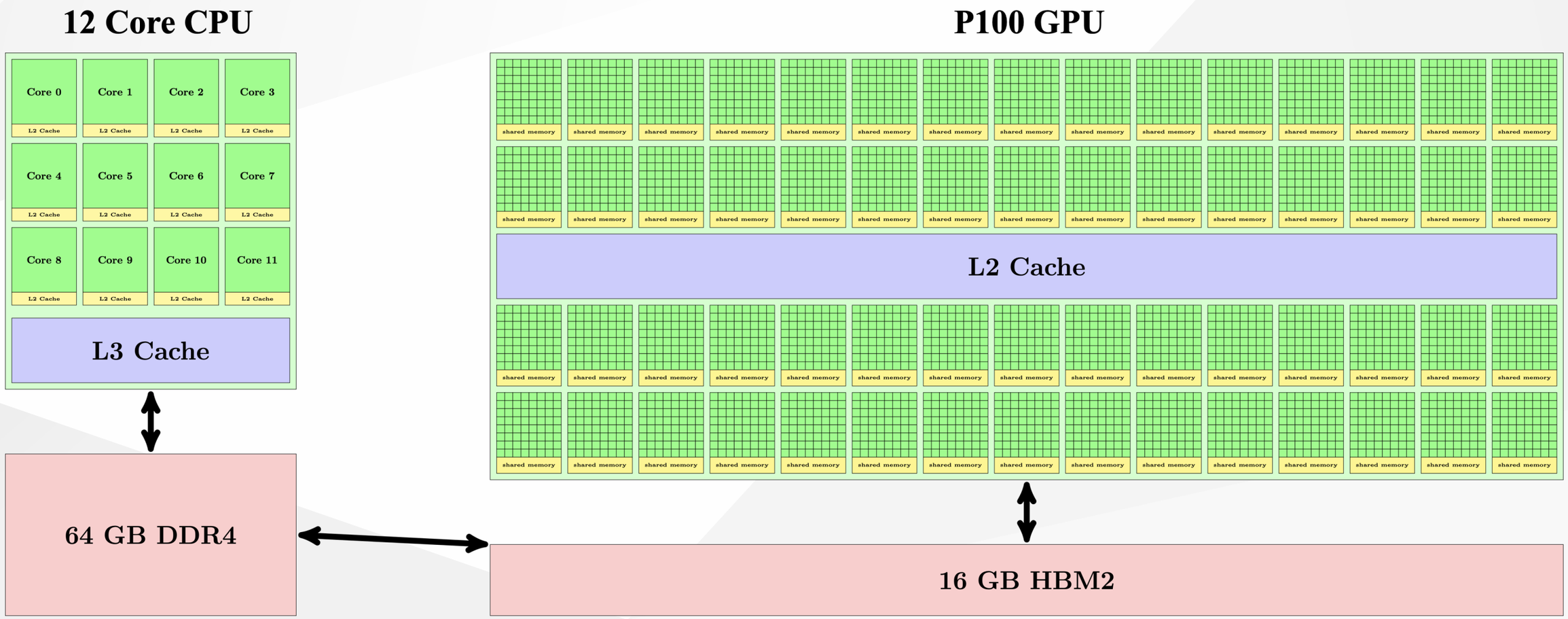


No GPU details visible to user

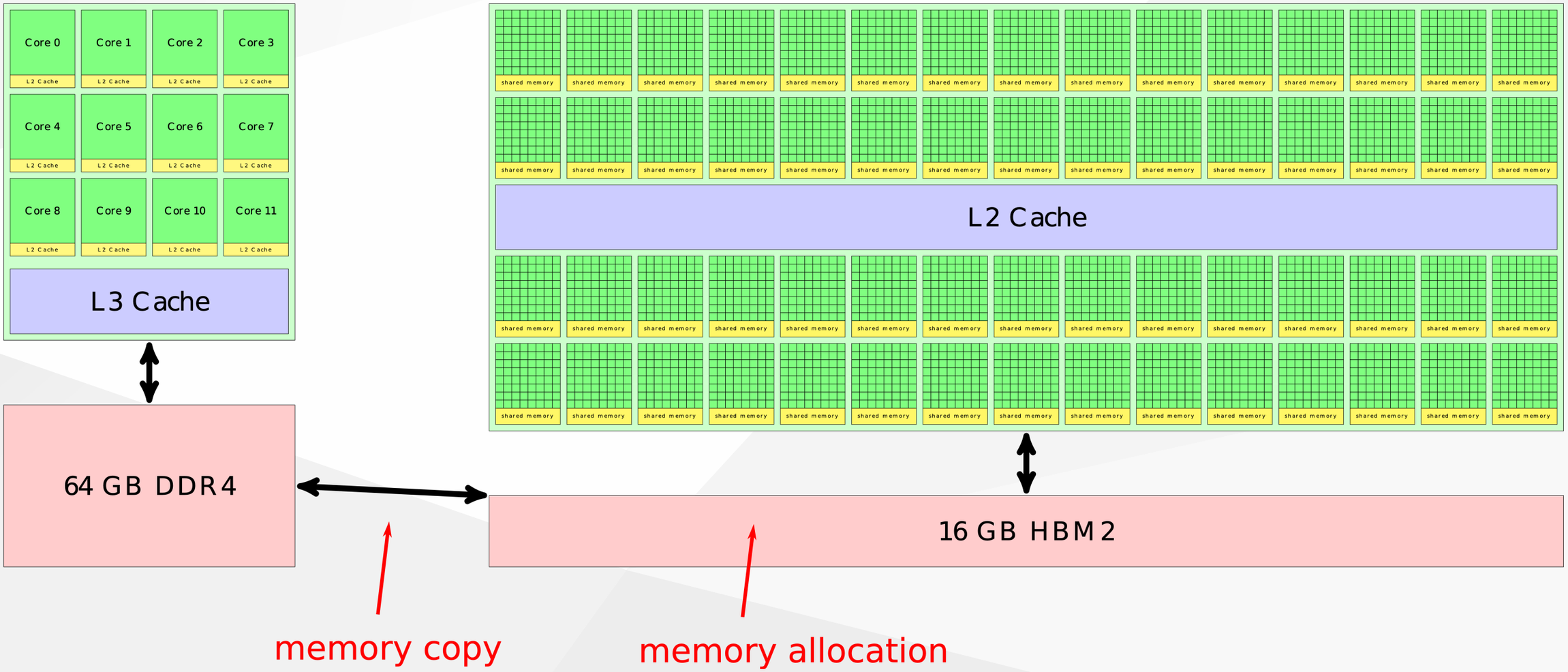
No GPU kernel code, but user manages GPU memory

Development of GPU kernel code

Hardware & Memory on a Piz Daint Node



Hardware & Memory on a Piz Daint Node



Host & 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

hardware	bandwidth	remarks
host ↔ 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** 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 PCI-Express bus 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 `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?

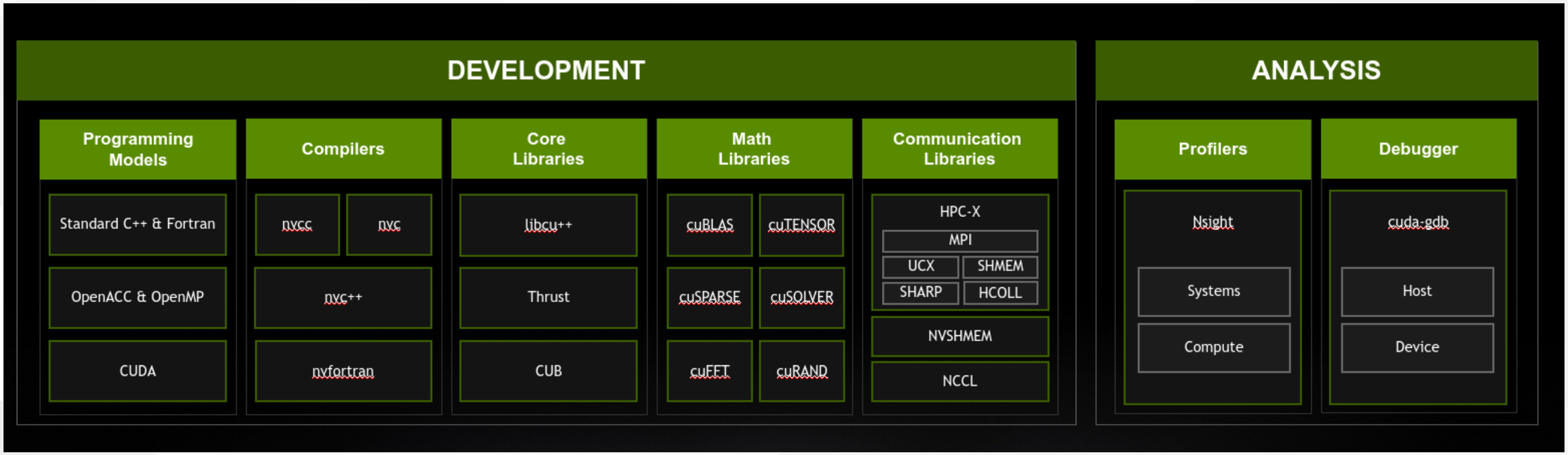
```
> srun nvprof -o explicit.nvvp --profile-from-start off -f ./explicit 25
> nvvp explicit.nvvp &
```

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...

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?