

Introduction to GPU Computing

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Motivation

- Massive parallelism and performance
- Good performance in relation to energy (FLOP/s per Watt)
- More and more compute clusters are becoming heterogeneous
- 9 out of the top 10 supercomputers feature GPUs
 - 6 NVIDIA
 - 2 AMD
 - 1 Intel
 - c.f. <https://www.top500.org/lists/top500/2024/06/>

CPU-GPU Comparison

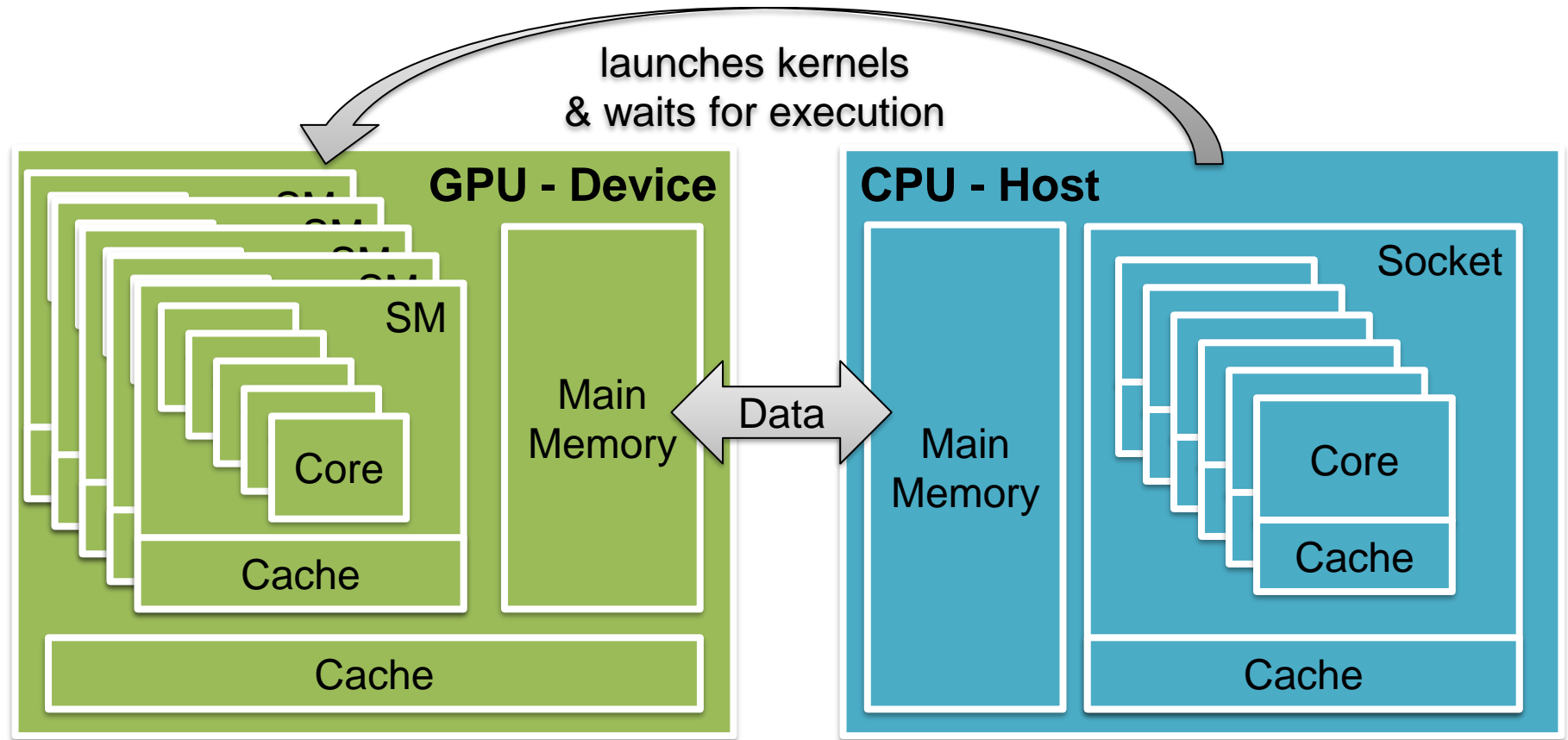
CPU

- Cores
 - Few but powerful
 - Memory
 - Large capacity
 - Latency optimized
- Ideal for irregular workload
- A small number of fast threads

GPU

- Cores
 - Many but less powerful
 - Memory
 - Small capacity
 - Bandwidth optimized
- Ideal for massively parallel structured computations

Simplified Architecture



Workflow

1. Initialize data on CPU
2. Copy data from CPU to GPU
3. Launch GPU kernels
4. Do independent work on CPU (optional)
5. Synchronize GPU
6. Copy data from GPU to CPU
7. Post-process data on CPU

Programming models

- Dedicated programming languages

- NVIDIA CUDA
- AMD HIP
- SYCL
- ...

```
__global__ void stream(size_t nx, double * src, double *
dest) {
    size_t i = blockIdx.x * blockDim.x + threadIdx.x;

    if (i < nx)
        dest[i] = src[i] + 1;
}

int main(int argc, char *argv[]) {
    double *src, *dest;
    cudaMallocManaged((void **) &src, sizeof(double) * nx);
    cudaMallocManaged((void **) &dest, sizeof(double) * nx);

    stream<<<(nx + 255) / 256, 256>>>(nx, src, dest);
    checkCudaError(cudaDeviceSynchronize());

    checkSolutionStream(src, nx);

    cudaFree(src);
    cudaFree(dest);
}
```

Programming models

- Dedicated programming languages
- Pragma-based approaches
 - OpenACC
 - OpenMP

```
int main(int argc, char *argv[]) {  
    auto src  = new double[nx];  
    auto dest = new double[nx];  
  
    #pragma omp target teams distribute parallel for data  
    map(from : src[0 : nx], to dest[0 : nx]) schedule(static)  
        for (int i = 0; i < nx; ++i)  
            dest[i] = src[i] + 1;  
  
    checkSolutionStream(src, nx);  
  
    delete[] src;  
    delete[] dest;  
}
```

Programming models

- Dedicated programming languages
- Pragma-based approaches
- Software layers
 - Kokkos
 - ...

```
int main(int argc, char *argv[]) {
    Kokkos::initialize(c, argv);
    {
        Kokkos::View<double *> src ("src", nx);
        Kokkos::View<double *> dest("dest", nx);

        Kokkos::parallel_for(Kokkos::RangePolicy<>(0, nx),
                             KOKKOS_LAMBDA(int i) {
                                 dest(i) = src(i) + 1;
                             });

        Kokkos::fence();

        checkSolutionStream(src.data(), nx);
    }
    Kokkos::finalize();
}
```


Programming models

- Dedicated programming languages
 - Full control – more evolved code for maximized performance potential
- Pragma-based approaches
 - Easy to integrate – if everything works as intended
- Software layers
 - Performance portability – ideally