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Introduction to GPUs in HPC

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2D and 3D Launch Configurations

Launch Configuration

- So far we have used one-dimensional launch configurations
  - threads in blocks indexed using `threadIdx.x`
  - blocks in a grid indexed using `blockIdx.x`
- Many kernels map naturally onto 2D and 3D indexing
  - e.g. matrix-matrix operations
  - e.g. stencils

Full Launch Configuration

Kernel launch dimensions can be specified with `dim3` structs

```
kernel<<<dim3 grid_dim, dim3 block_dim>>>(...);
```

- `dim3.x`, `dim3.y` and `dim3.z` specify the launch dimensions
- can be constructed with 1, 2 or 3 dimensions
- unspecified `dim3` dimensions are set to 1

launch configuration examples

```
// 1D: 128x1x1 for 128 threads
dim3 a(128);
// 2D: 16x8x1  for 128 threads
dim3 b(16, 8);
// 3D: 16x8x4  for 512 threads
dim3 c(16, 8, 4);
```

The `threadIdx`, `blockDim`, `blockIdx` and `gridDim` can be treated like 3D vectors via the `.x`, `.y` and `.z` members.

matrix addition example

```
__global__
void MatAdd(float *A, float *B, float *C, int n) {
    int i = blockIdx.x * blockDim.x + threadIdx.x;
    int j = blockIdx.y * blockDim.y + threadIdx.y;
    if(i<n && j<n) {
        auto pos = i + j*n;
        C[pos] = A[pos] + B[pos];
    }
}
int main() {
    // ...
    dim3 threadsPerBlock(16, 16);
    dim3 numBlocks(n / threadsPerBlock.x, n / threadsPerBlock.y);
    MatAdd<<<numBlocks, threadsPerBlock>>>(A, B, C);
    // ...
}
```

Exercise: Launch Configuration

- Write the 2D diffusion stencil in `diffusion/diffusion2d.cu`
- Set up 2D launch configuration in the main loop
- Draw a picture of the solution to validate it
  - a plotting script is provided for visualizing the results
  - use a small domain for visualization

```
# build and run after writing code
cd diffusion
srun diffusion2d 8 1000000

# do the plotting
module load daint/gpu
module load Python/2.7.12-CrayGNU-2016.11
python plotting.py
```

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Using MPI with GPUs

What is MPI

MPI (**Message Passing Interface**) is a standardised library for message passing

- Highly portable: it is implemented on every HPC system available today.
- Has C, C++ and Fortran bindings.
- Supports point to point communication
  - `MPI_Send`, `MPI_Recv`, `MPI_Sendrecv`, etc.
- Supports global collectives
  - `MPI_Barrier`, `MPI_Gather`, `MPI_Reduce`, etc.

When you start an MPI application

- N copies of the application are launched.
- Each copy is given a **rank** $\in \{0, 1, \ldots, N-1\}$.

A basic MPI application

Example MPI application myapp.cpp

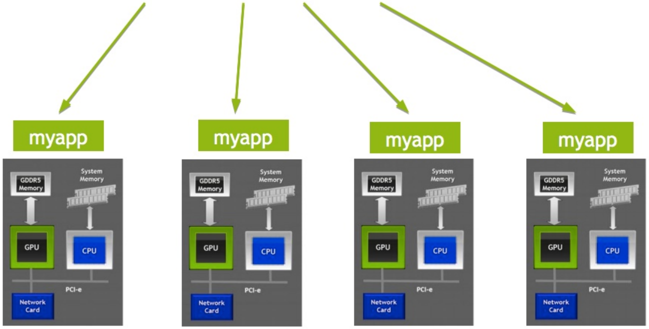
```
#include <mpi.h>
#include <unistd.h>
#include <cstdio>

int main(int argc, char** argv) {
    // initialize MPI on this rank
    MPI_Init(&argc, &argv);
    // get information about our place in the world
    int rank, size;
    MPI_Comm_rank(MPI_COMM_WORLD, &rank);
    MPI_Comm_size(MPI_COMM_WORLD, &size);
    // print a message
    char name[128]; gethostname(name, sizeof(name));
    printf("hello world from %d of %d on %s\n", rank, size, name);
    // close down MPI
    MPI_Finalize();
    return 0;
}
```

MPI applications are compiled with a **compiler wrapper**:

```
> CC myapp.cpp -o myapp # the Cray C++ wrapper is CC
```

Running our basic MPI application

```
# run myapp 4 ranks (-n) on 4 nodes (-N)
> srun -n4 -N4 ./myapp
hello world from 0 of 4 on nid02117
hello world from 1 of 4 on nid02118
hello world from 2 of 4 on nid02119
hello world from 3 of 4 on nid02120
```



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MPI with data in device memory

We use GPUs to parallelize on-node computation

- and probably MPI for communication between nodes

To use with data that is in buffers in GPU memory:

1. allocate buffers in host memory
2. manually copy from device$\rightarrow$host memory
3. perform MPI communication with host buffers
4. copy received data from host$\rightarrow$device memory

This approach can be very fast:

- have a CPU thread dedicated to asynchronous host$\leftrightarrow$device and MPI communication

GPU-aware MPI

GPU-aware MPI implementations can automatically handle MPI transactions with pointers to GPU memory

- MVAPICH 2.0
- OpenMPI since version 1.7.0
- Cray MPI

How it works

- Each pointer passed to MPI is checked to see if it is in host or device memory. If not set, MPI assumes that all pointers are to host memory, and your application will probably crash with segmentation faults
- Small messages between GPUs (up to ≈8 k) are copied directly with **RDMA**
- Larger messages are **pipelined** via host memory

How to use G2G communication

- Set the environment variable `export MPICH_RDMA_ENABLED_CUDA=1`
  - If not set, MPI assumes that all pointers are to host memory, and your application will probably crash with segmentation faults
- Experiment with the environment variable `MPICH_G2G_PIPELINE`
  - Sets the maximum number of 512 kB message chunks that can be in flight (default 16)

MPI with G2G example

```
MPI_Request srequest, rrequest;
auto send_data = malloc_device<double>(100);
auto recv_data = malloc_device<double>(100);

// call MPI with GPU pointers
MPI_Irecv(recv_data, 100, MPI_DOUBLE, source, tag, MPI_COMM_WORLD,
     &rrequest);
MPI_Isend(send_data, 100, MPI_DOUBLE, target, tag, MPI_COMM_WORLD,
     &srequest);
```

Capabilities and Limitations

- Support for most MPI API calls (point-to-point, collectives, etc)
- Robust support for common MPI API calls
  - i.e. point-to-point operations
- No support for user-defined MPI data types

Exercise: MPI with G2G

- 2D stencil with MPI in `diffusion/diffusion2d_mpi.cu`
- Implement the G2G version
  1. can you observe any performance differences between the two?
  2. why are we restricted to just 1 MPI rank per node?
- Implement a version that uses managed memory
  - what happens if you don't set `MPICH_RDMA_ENABLED_CUDA`?

```
# load modules require to compile MPI
module swap PrgEnv-cray PrgEnv-gnu
module load cudatoolkit

# launch with 2 MPI ranks
MPICH_RDMA_ENABLED_CUDA=1 srun --reservation=Pascal2day -p jalet
        -C gpu -n2 -N2 diffusion2d_mpi.cuda 8

# plot the solution
module load python/2.7.6
python plotting.py

# once it gets the correct results:
sbatch job.batch
```

Exercises: 2D Diffusion with MPI Results

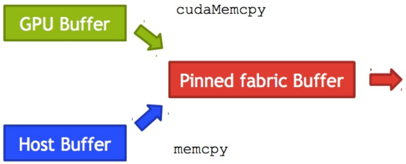
Time for 1000 time steps 128×16,382 on K20X GPUs

nodes	G2G off	G2G on
1	0.479	0.479
2	0.277	0.274
4	0.183	0.180
8	0.152	0.151
16	0.167	0.117

Using Unified Memory with MPI

- To pass a managed pointer to MPI you must use a GPU-aware MPI distribution.
- Even if the managed memory is on the host at time of calling.

- The MPI implementation uses page-locked (pinned) memory for RDMA.
- If not aware of unified memory you get
  - if lucky: crashes.
  - if unlucky: infuriating bugs.



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