Pázmány Péter Catholic University
Faculty of Information Technology and Bionics

# Accelerated Computing - GPUs and OpenMP

Lecture 7

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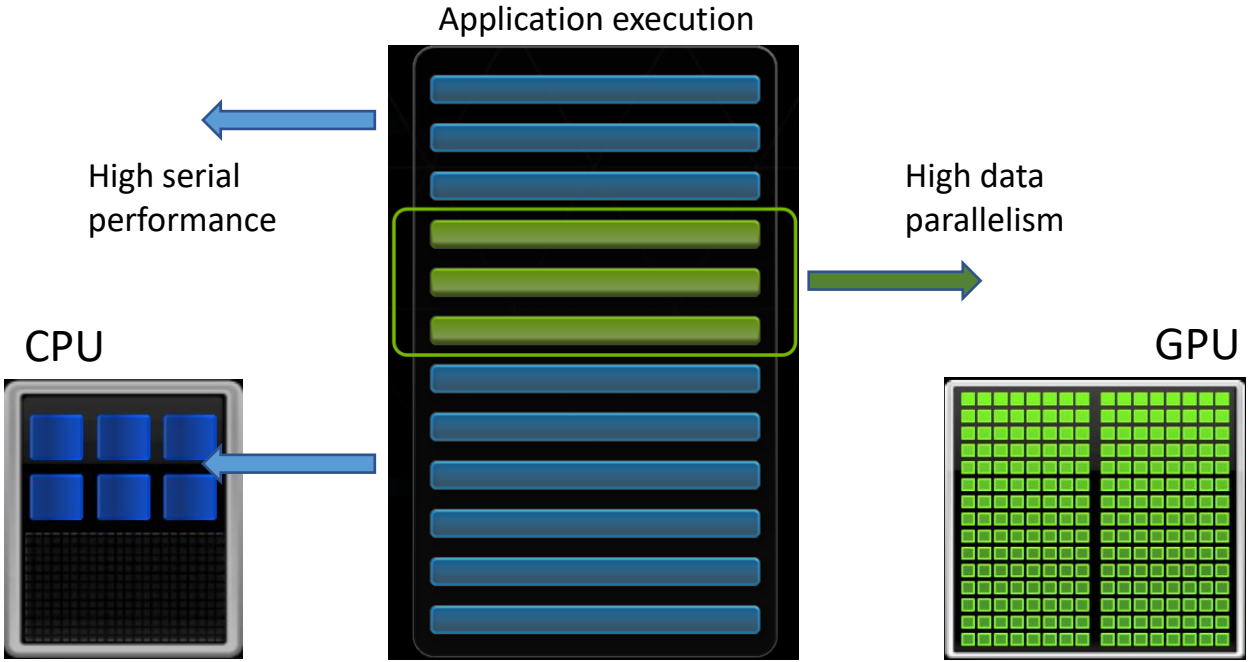
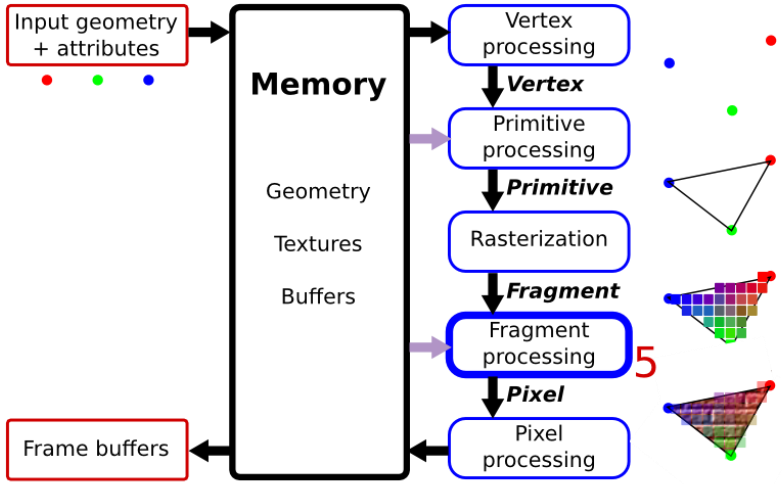
# Accelerated computing



# GPUs

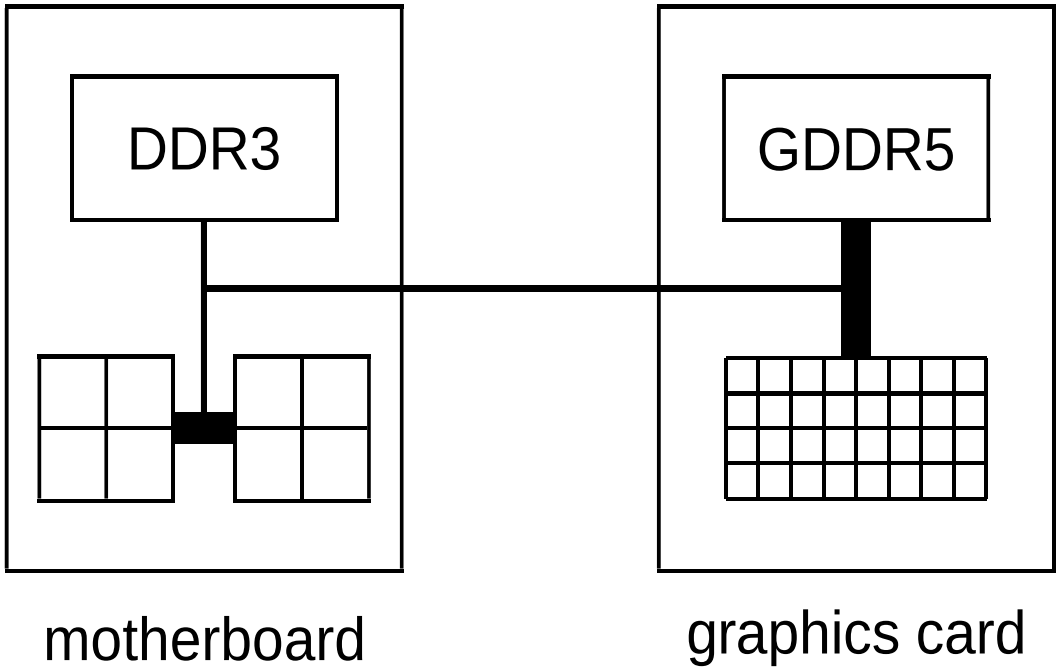
- GPUs are data-parallel computing units
- Origins:
  - Late 90's 3Dfx Voodoo
  - 2000's ATI vs. NVIDIA
  - Graphics oriented, fixed pipelines




# Modern GPUs

- Pipelines became more programmable
  - 2007 – CUDA released
  - General purpose programmability
- Still very much driven by the needs of graphics applications (and AI)
- Increasingly similar to multi-core CPUs with wide vector units

# CPU-GPU system




# GPUs

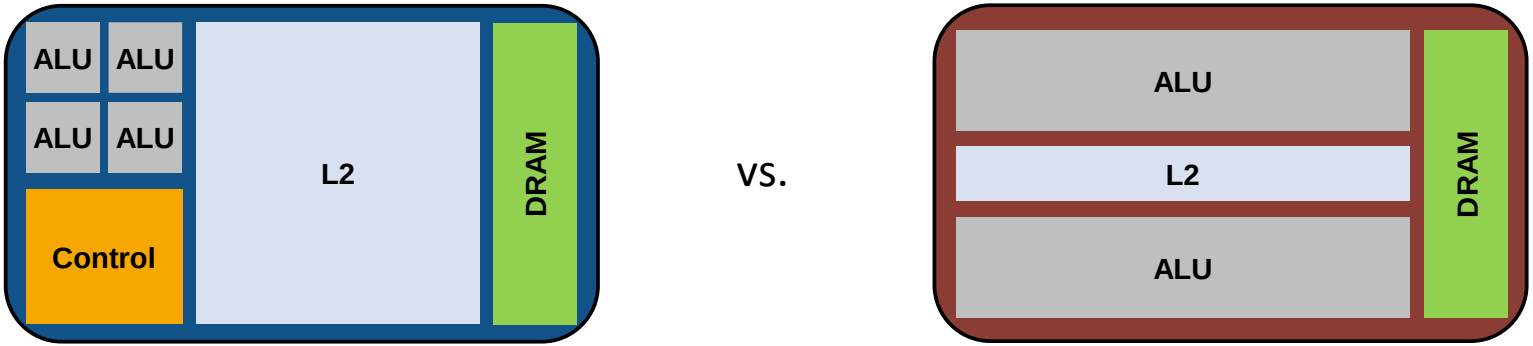
- Up to 10000 “cores” on a chip
- Simplified logic (no out-of-order execution) – most of the chip is devoted to floating-point computation
- Arranged as multiple units with each one effectively being a vector unit, with all cores doing the same thing
- Very high bandwidth to graphics memory (up to 3000 GB/s)
- Not general purpose – graphics and other highly data-parallel applications


# GPU clusters

- People build large supercomputers using GPUs
- One single/dual-socket CPU machine with 1-4 GPUs
  - Like the one you'll be working on
- Interconnected with Infiband – light fibre, with up to 25 Gbit/s (vs. 1 Gbit/s Ethernet)
- Summit – 27.648 GPUs
  - 200 Pflops
  - 13 MW
- Frontier – 37.888 GPUs
  - 1.1 Exaflops
  - 21 MW

# Performance of GPUs

- CPUs are latency oriented: do one thing really fast
  - Caches, Out-of-order execution, etc.
- GPUs are throughput oriented: do a lot of things fast
  - Execution of individual tasks is still slow
  - Relies on massive multi-threading:
    - Up to 16 threads per core
    - While one waits (e.g. for memory), others can work
    - Zero overhead context switching



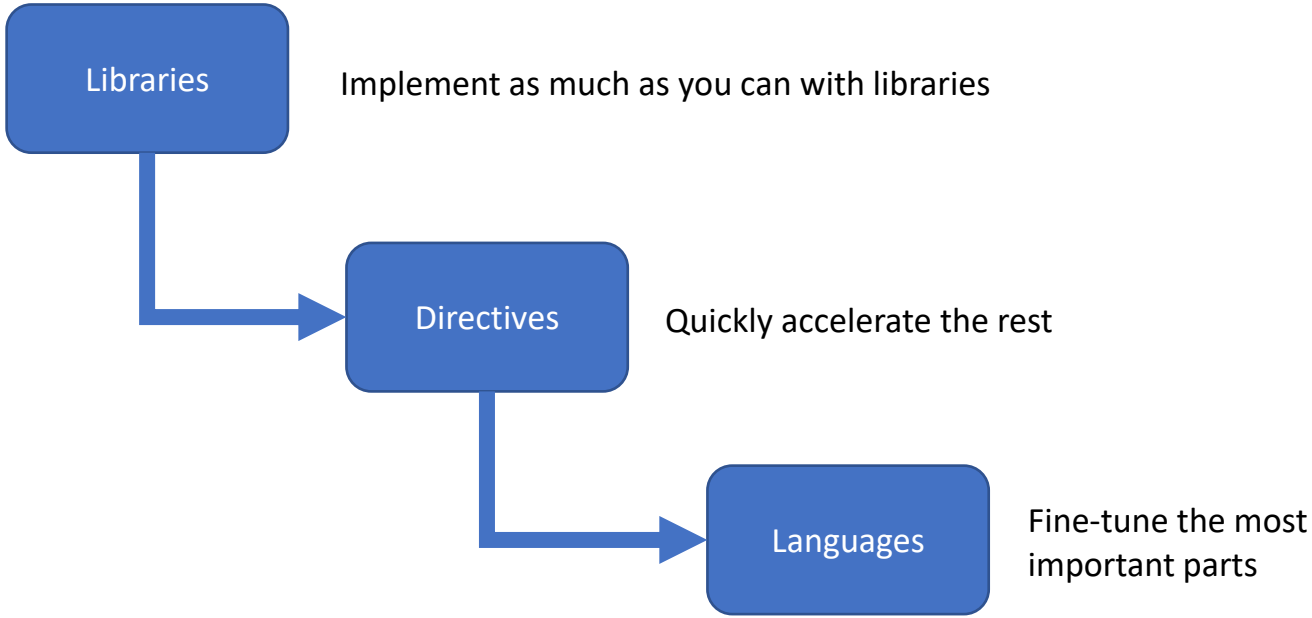

# How do we program GPUs

- GPUs have  a very complicated hardware architecture
  - Significant changes between generations
- To get every last bit of performance, really low level programming is required
  - Before 2007, people used shader languages
  - CUDA was introduced in 2007 – NVIDIA only
  - OpenCL was introduced in 2009 – other vendors too
- These are very low-level approaches!

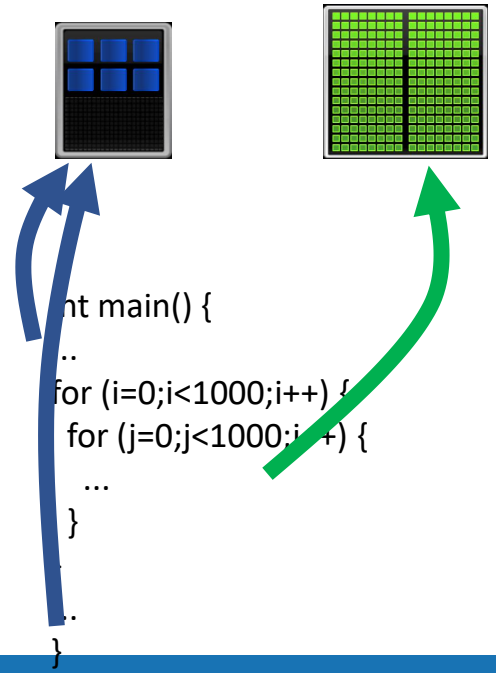
# Simplicity & Performance


- Accelerated Libraries
  - Little or no code change for standard libraries
  - Limited in what the library offers
- Compiler Directives
  - High level: Based on existing languages; simple and familiar
  - High Level: Performance may not be optimal
- Parallel Language Extensions
  - Expose low-level details for maximum performance
  - Often more difficult to learn and more time consuming to implement

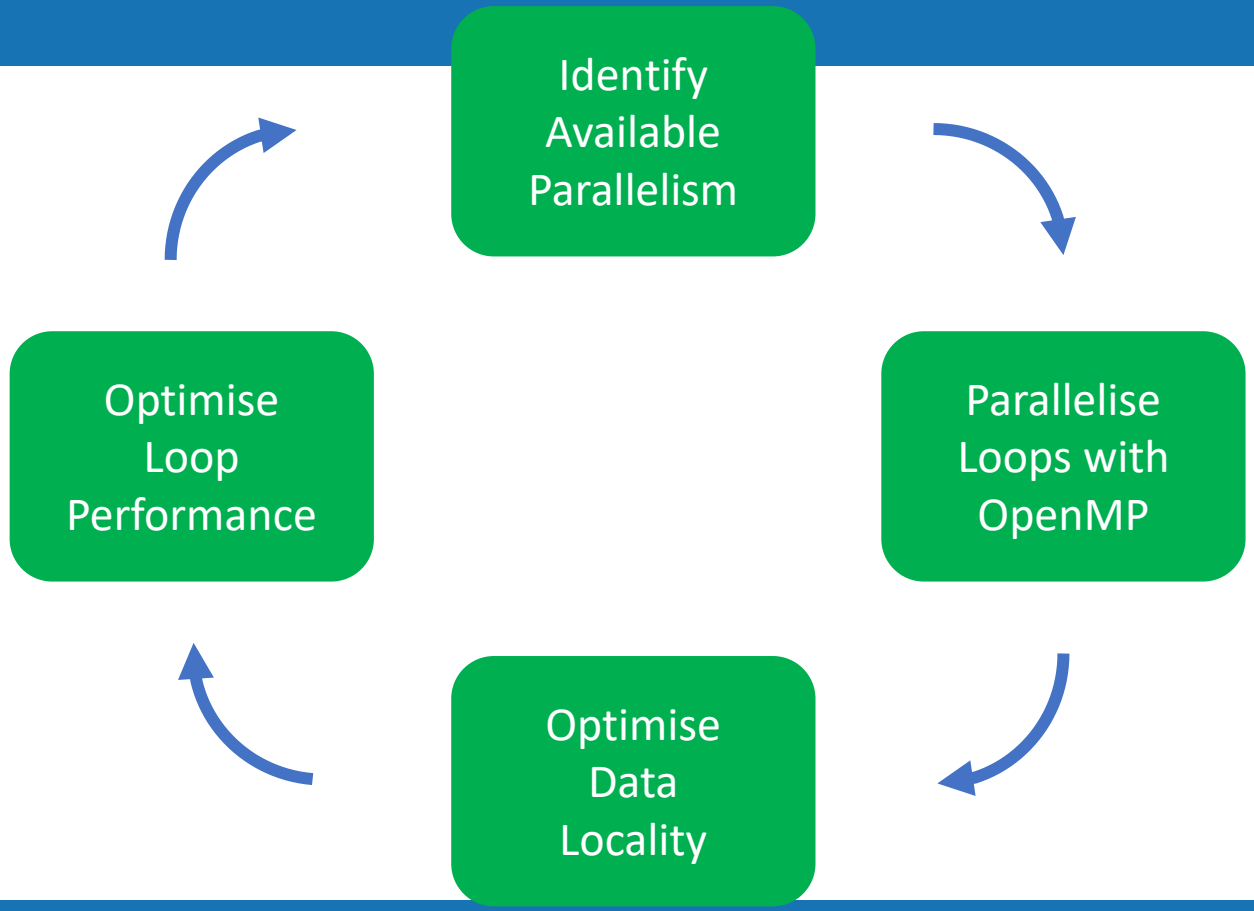
# Code for simplicity and performance



# GPU Directives




- Insert portable compiler directives
- Compiler parallelizes code and manages data movement
- Programmer optimizes incrementally
- Designed for multi-core CPUs, GPUs & many-core Accelerators


Identify Available Parallelism
Parallelise Loops with OpenMP
Optimise Data Locality
Optimise Loop Performance

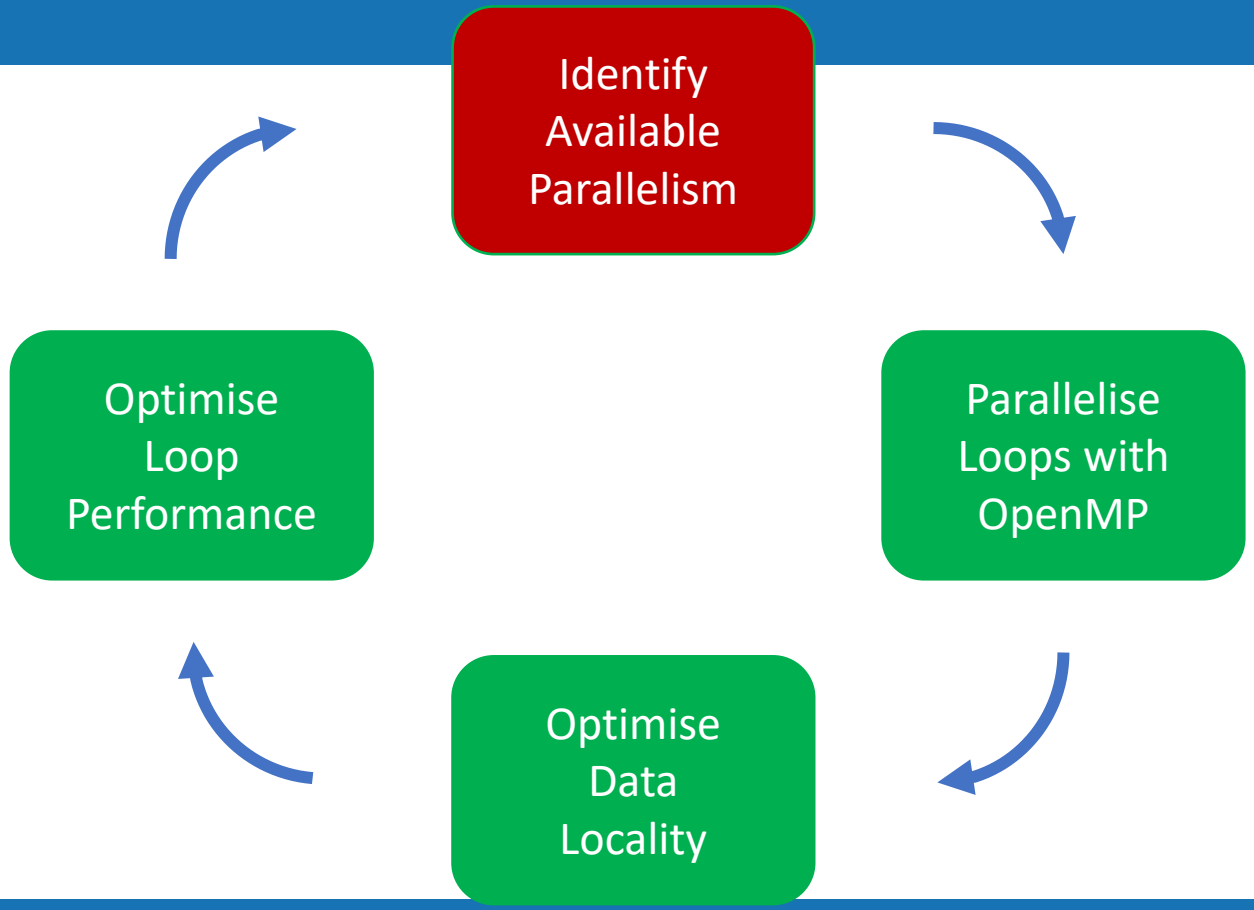
# Our laplace equation solver

```
while ( error > tol && iter < iter_max ) {
 error = 0.0;
 for( int i = 1; i < imax+1; i++ ) {
  for( int j = 1; j < jmax+1; j++) {
   Anew[j*(imax+2)+i] = 0.25f * (
                                A[(j+1) *(imax+2)+i] +
                                A[(j-1) *(imax+2)+i] +
                                A[j*(imax+2)+i-1] +
                                A[j*(imax+2)+i+1]);
   error = fmax( error, fabs(Anew[...]-A[...]));
  }
 }
 for( int i = 1; i < imax+1; i++ )
  for( int j = 1; j < jmax+1; j++)
   A[j*(imax+2)+i] = Anew[j*(imax+2)+i];
 if(iter % 100 == 0)
  printf("%5d, %0.6f\n", iter, error);
 iter++;
}
```

- Iterate for iter_max
- Iterate across grid
- Compute new value
- Reduce error
- Copy input/output
- Print residual


# Exercise

- Compile the laplace2d.cpp using the Cray compilers
- To compile:
  - `CC -Ofast -fopenmp laplace2d.cpp -o laplace_cpu`
- To run:
  - `salloc -p cpu -c 16 --mem-per-cpu=2000 --time=00:05:00 srun --ntasks=1 ./laplace_cpu`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# Identify parallelism

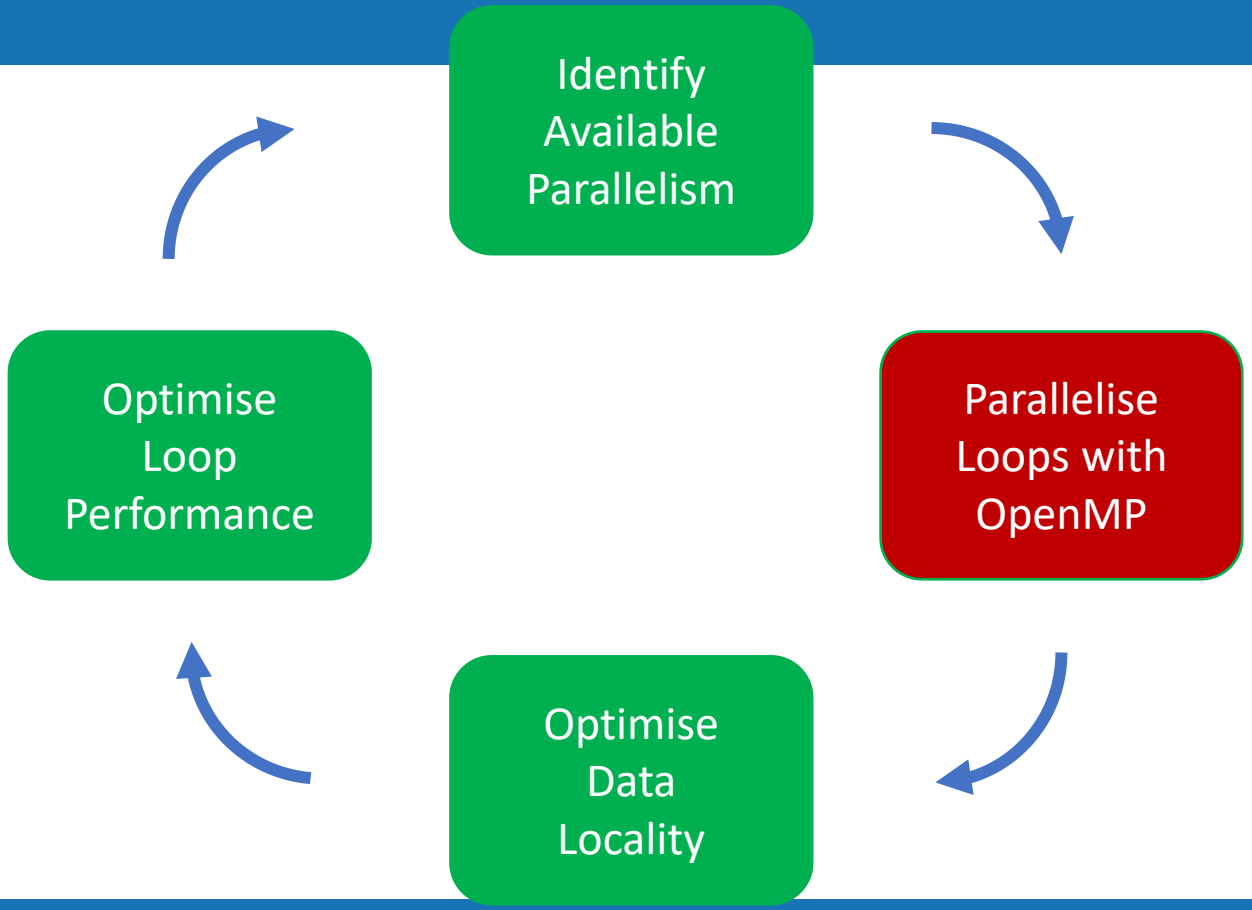
```
while ( error > tol && iter < iter_max ) {
 error = 0.0;
 for( int i = 1; i < imax+1; i++ ) {
  for( int j = 1; j < jmax+1; j++) {
   Anew[j*(imax+2)+i] = 0.25f * (
                                A[(j+1) *(imax+2)+i] +
                                A[(j-1) *(imax+2)+i] +
                                A[j*(imax+2)+i-1] +
                                A[j*(imax+2)+i+1]);
   error = fmax( error, fabs(Anew[...]-A[...]));
  }
 }
 for( int i = 1; i < imax+1; i++ )
  for( int j = 1; j < jmax+1; j++)
   A[j*(imax+2)+i] = Anew[j*(imax+2)+i];
 if(iter % 100 == 0)
  printf("%5d, %0.6f\n", iter, error);
 iter++;
}
```

Data dependency

Independent iterations

Reduction

Independent iterations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# OpenMP directive syntax

- C/C++ - very similar to OpenMP CPU parallelisation

  #pragma omp target [clause [,] clause] ...]

- target – identifies a block of code that should be offloaded to a “target” device - becomes a “kernel”
- teams distribute – chunk up execution between larger “cores” on the GPU
- parallel for – parallelize iterations of for loop across different threads within the “core” on the GPU

```
#pragma target teams distribute parallel for
for(int i=0; i<N; i++) {
    y[i] = a*x[i]+y[i];
}
```

**Kernel**: A function that runs in parallel on the GPU

# Parallelising with OpenMP

```
while ( error > tol && iter < iter_max ) {
 error = 0.0;
#pragma omp target teams distribute parallel for reduction(max:error) \
      map(A[0:(imax+2)*(jmax+2)]) map(Anew[0:(imax+2)*(jmax+2)])
 for( int i = 1; i < imax+1; i++ ) {
  for( int j = 1; j < jmax+1; j++) {
   Anew[j*(imax+2)+i] = 0.25f * (
                                  A[(j+1) *(imax+2)+i] +
                                  A[(j-1) *(imax+2)+i] +
          A[j*(imax+2)+i-1] +
                                  A[j*(imax+2)+i+1]);
    error = fmax( error, fabs(Anew[...]-A[...]));
  }
 }
#pragma omp target teams distribute parallel for \
      map(A[0:(imax+2)*(jmax+2)]) map(Anew[0:(imax+2)*(jmax+2)])
 for( int i = 1; i < imax+1; i++ )
  for( int j = 1; j < jmax+1; j++)
   A[j*(imax+2)+i] = Anew[j*(imax+2)+i];
 if(iter % 100 == 0)
  printf("%5d, %0.6f\n", iter, error);
 iter++;
}
```

Parallelise loop

Parallelise loop

# Compiling with OpenMP

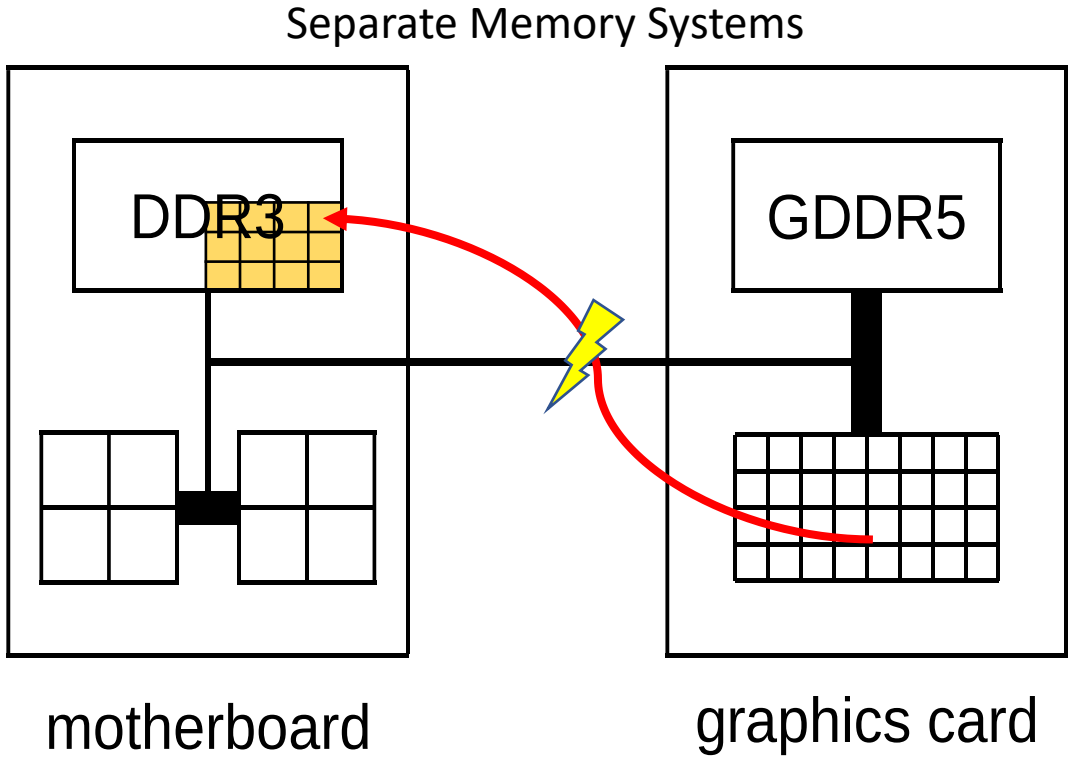
module load craype-accel-nvidia80

module load craype-accel-nvidia80
CC -Ofast laplace2d.cpp -o laplace -fopenmp –lcudart
srun -p gpu --gres=gpu:1 --ntasks=1 --time=00:05:00 --mem=40G ./laplace

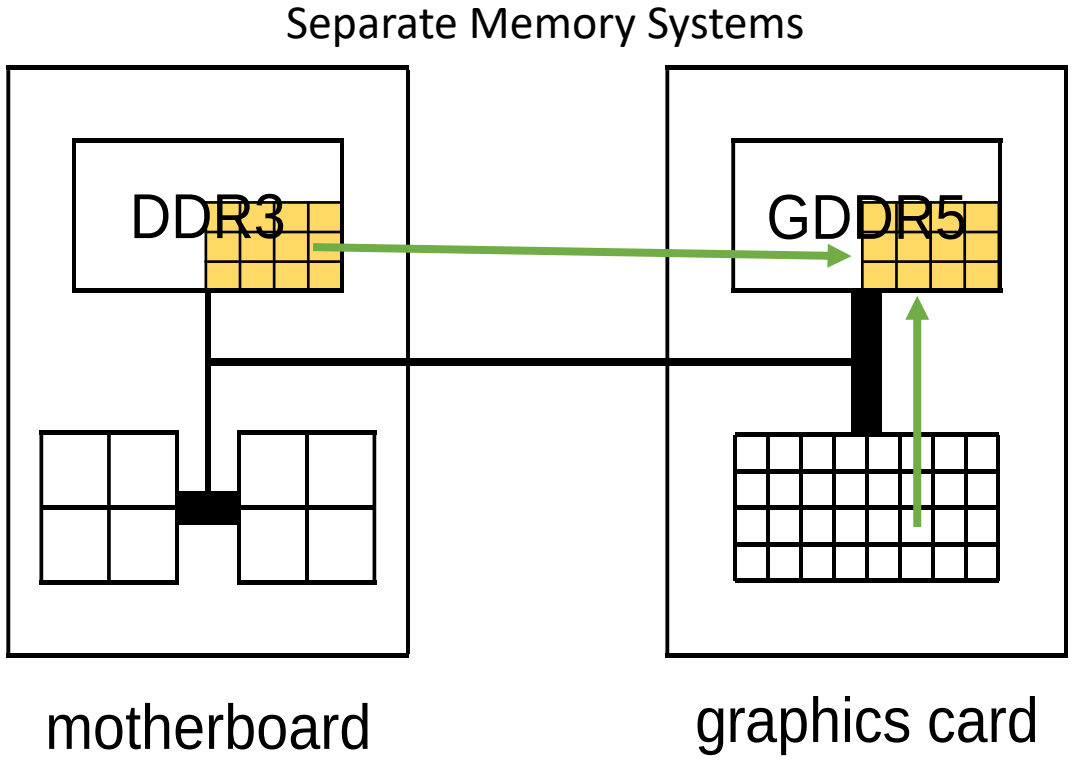
export CRAY_ACC_DEBUG=1
srun -p gpu --gres=gpu:1 --ntasks=1 --time=00:05:00 --mem=40G ./laplace

ACC: Transfer 3 items (to acc 268697672 bytes, to host 0 bytes) from laplace2d.cpp:62
ACC: Execute kernel __omp_offloading_20ea7bcc_c001c75b_main_l62 from laplace2d.cpp:62
ACC: Transfer 3 items (to acc 0 bytes, to host 268697672 bytes) from laplace2d.cpp:62
ACC: Transfer 2 items (to acc 268697664 bytes, to host 0 bytes) from laplace2d.cpp:72
ACC: Execute kernel __omp_offloading_20ea7bcc_c001c75b_main_l72_cce$noloop$form from laplace2d.cpp:72
ACC: Transfer 2 items (to acc 0 bytes, to host 268697664 bytes) from laplace2d.cpp:72

# CPU-GPU system

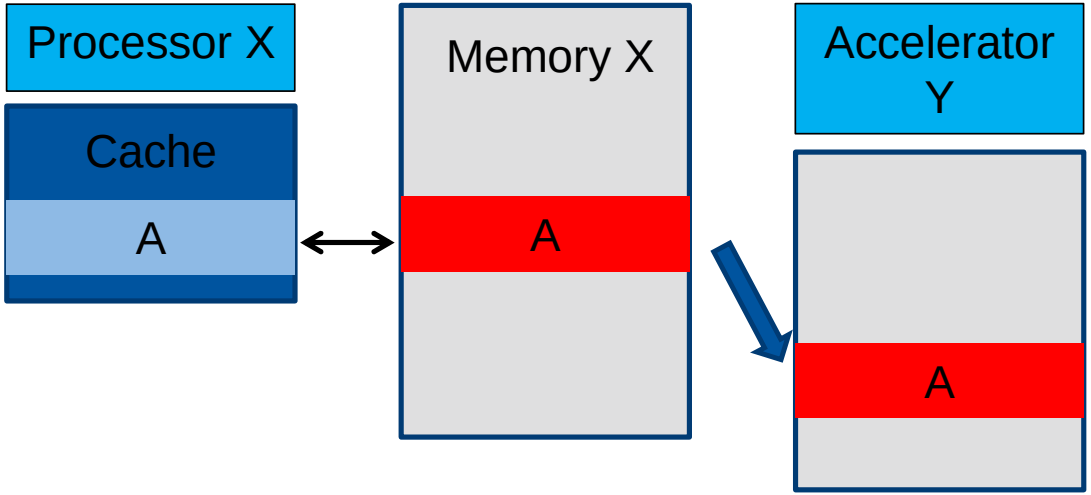


# CPU-GPU system



# CPU and GPU arrays

- OpenMP has to copy our CPU arrays to the GPU
  - But it does not know how big they are
  - Extra clauses on top of acc parallel loop:
  - map(A[0:((imax+2) * (jmax+2))]) map(Anew[0:((imax+2) * (jmax+2))])




# Exercise: Performance

- Measure performance:
  - serial
  - multi-core CPU with OpenMP
  - GPU with OpenMP

- Much slower with OpenMP on GPU

# Why so bad? – Data transfers!

```
while ( error > tol && iter < iter_max ) {
```

A,Anew on host → A,Anew on device

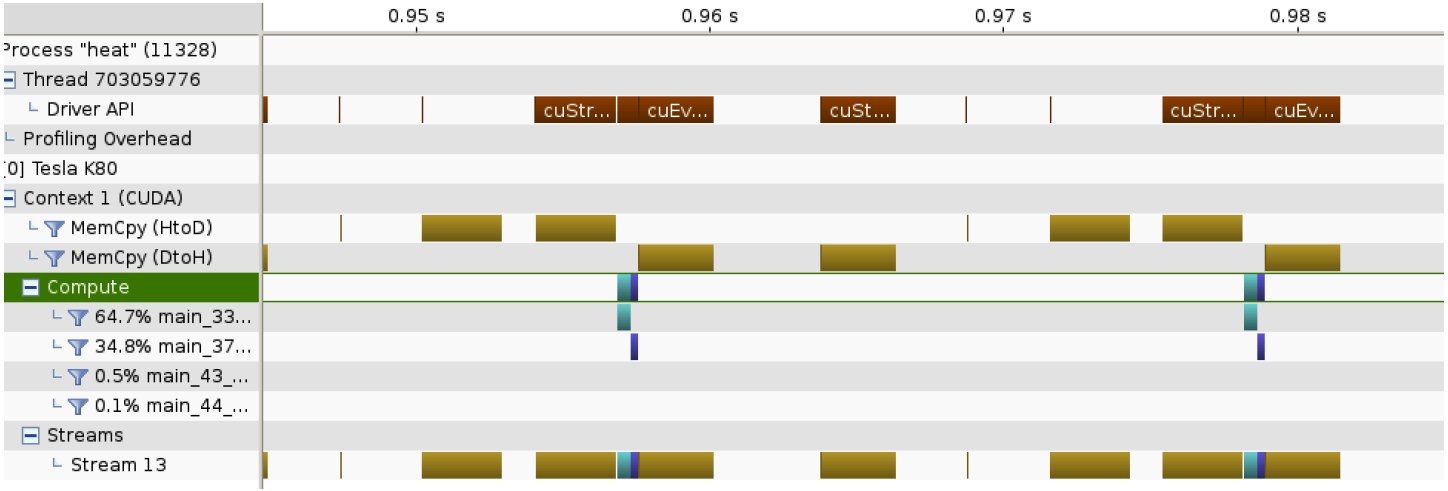
```
#pragma omp target distribute parallel for reduction(max:error) \
      map(A[0:(imax+2)*(jmax+2)]) map(Anew[0:(imax+2)*(jmax+2)])
 for( int i = 1; i < imax+1; i++ ) {
  for( int j = 1; j < jmax+1; j++) {
   Anew[j*(imax+2)+i] = 0.25f * (
                                A[(j+1) *(imax+2)+i] +
                                A[(j-1) *(imax+2)+i] +
          A[j*(imax+2)+i-1] +
                                A[j*(imax+2)+i+1]);
   error = fmax( error, fabs(Anew[...]-A[...]));
  }
 }
...
```

A,Anew on device → A,Anew on host

**Happens every time!!**

# Profiling the application

- Reduce overall iteration count to ~100
- Use the NVIDIA Visual Profiler (requires X forwarding):
  - nvvp ./laplace2d &



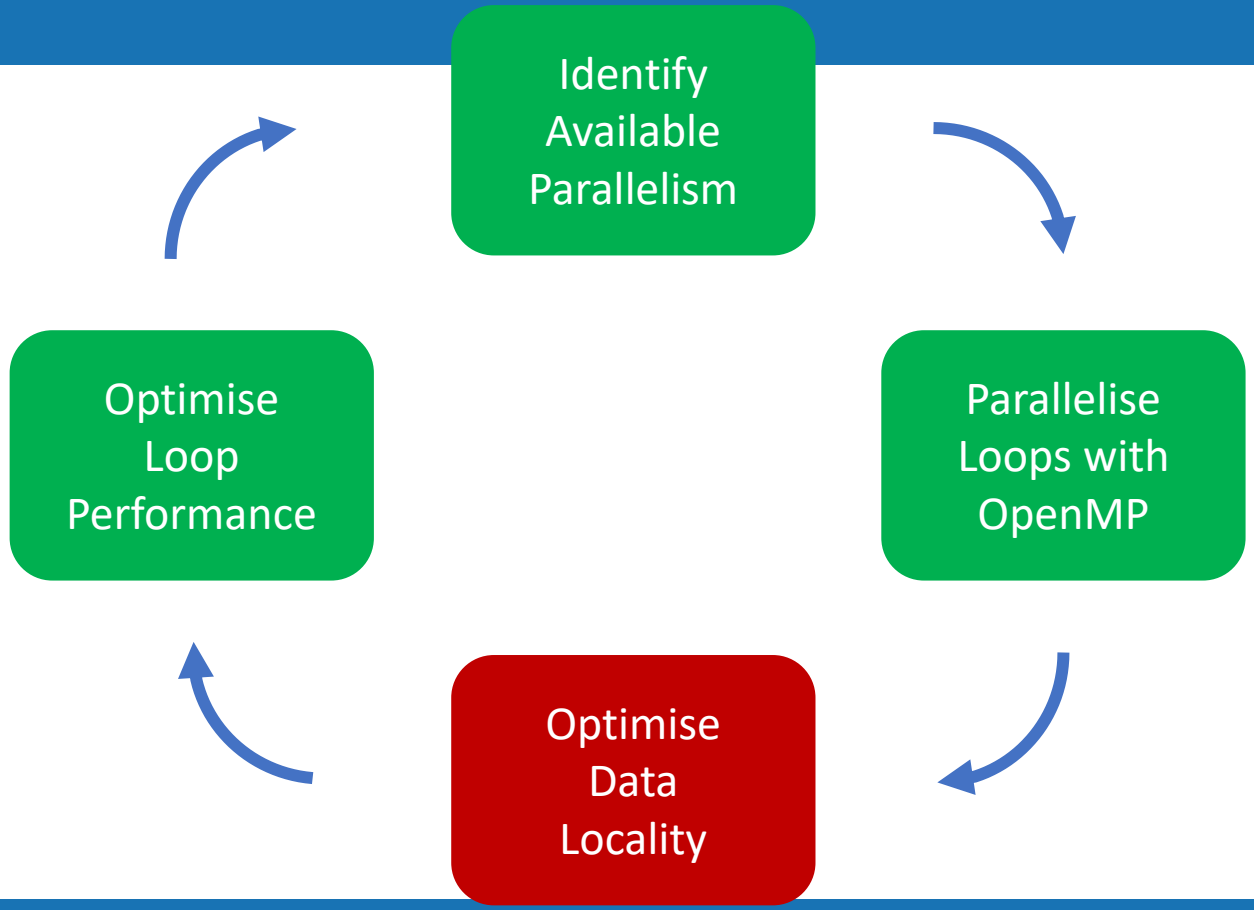
# Identifying data locality

```
while ( error > tol && iter < iter_max ) {
 error = 0.0;
#pragma omp target distribute parallel for reduction(max:error) \
 map(A[0:((imax+2) * (jmax+2))]) \
 map(Anew[0:((imax+2) * (jmax+2))])

 for( int i = 1; i < imax+1; i++ ) {
  for( int j = 1; j < jmax+1; j++) {
   Anew[j*(imax+2)+i] = 0.25f * (
                                 A[(j+1) *(imax+2)+i] +
                                 A[(j-1) *(imax+2)+i] +
        A[j*(imax+2)+i-1] +
                                 A[j*(imax+2)+i+1]);
   error = fmax( error, fabs(Anew[...]-A[...]));
  }
 }
#pragma omp target distribute parallel for \
map(A[0:((imax+2) * (jmax+2))]) map(Anew[0:((imax+2) * (jmax+2))])
 for( int i = 1; i < imax+1; i++ )
  for( int j = 1; j < jmax+1; j++)
   A[j*(imax+2)+i] = Anew[j*(imax+2)+i];
 if(iter % 100 == 0)
  printf("%5d, %0.6f\n", iter, error);
 iter++;
}
```

Does the CPU need the data between these loop nests?

Does the CPU need the data between iterations?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# Defining data regions

- The **`data`** construct defines a region of code in which GPU arrays remain on the GPU and are shared among all kernels in that region.

```
#pragma omp target data
{
#pragma omp target distribute
...
#pragma omp target distribute
...
}
```

Arrays used within the data region will remain on the GPU until the end of the data region.


# Data clauses

- `map(list)` - Allocates memory on GPU and copies data from host to GPU when entering region and copies data to the host when exiting region.
- `map(tofrom:list)` – same as above
- `map(to:list)` - Allocates memory on GPU and copies data from host to GPU when entering region.
- `map(from:list)` - Allocates memory on GPU and copies data to the host when exiting region.
- `map(alloc:list)` - Allocates memory on GPU but does not copy


# Array sharing

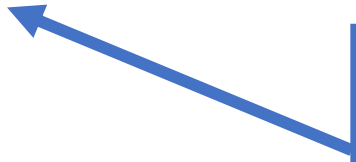
- Some compilers try to determine the size of arrays automatically – check compiler feedback! (NVIDIA nvhpc)
- Sometimes cannot – you have to explicitly specify the shape!

```
#pragma omp target data map(to:a[0:size]) map(from:b[s/4:3*s/4])
```

Note: data clauses can be used on `data`, `target`

# Managing data

```
#pragma omp target data \
 map(A[0:((imax+2) * (jmax+2))]) \
 map(Anew[0:((imax+2) * (jmax+2))])
while ( error > tol && iter < iter_max ) {
 error = 0.0;
#pragma omp target distribute parallel for reduction(max:error)
 for( int i = 1; i < imax+1; i++ ) {
  for( int j = 1; j < jmax+1; j++) {
   Anew[i][j] = 0.25f * ( A[i][j+1] + A[i][j-1]
              + A[i-1][j] + A[i+1][j]);
   error = fmax( error, fabs(Anew[i][j]-A[i][j]));
  }
 }
#pragma omp target distribute parallel for
 for( int i = 1; i < imax+1; i++ )
  for( int j = 1; j < jmax+1; j++)
   A[i][j] = Anew[i][j];
 if(iter % 100 == 0)
  printf("%5d, %0.6f\n", iter, error);
 iter++;
}
```

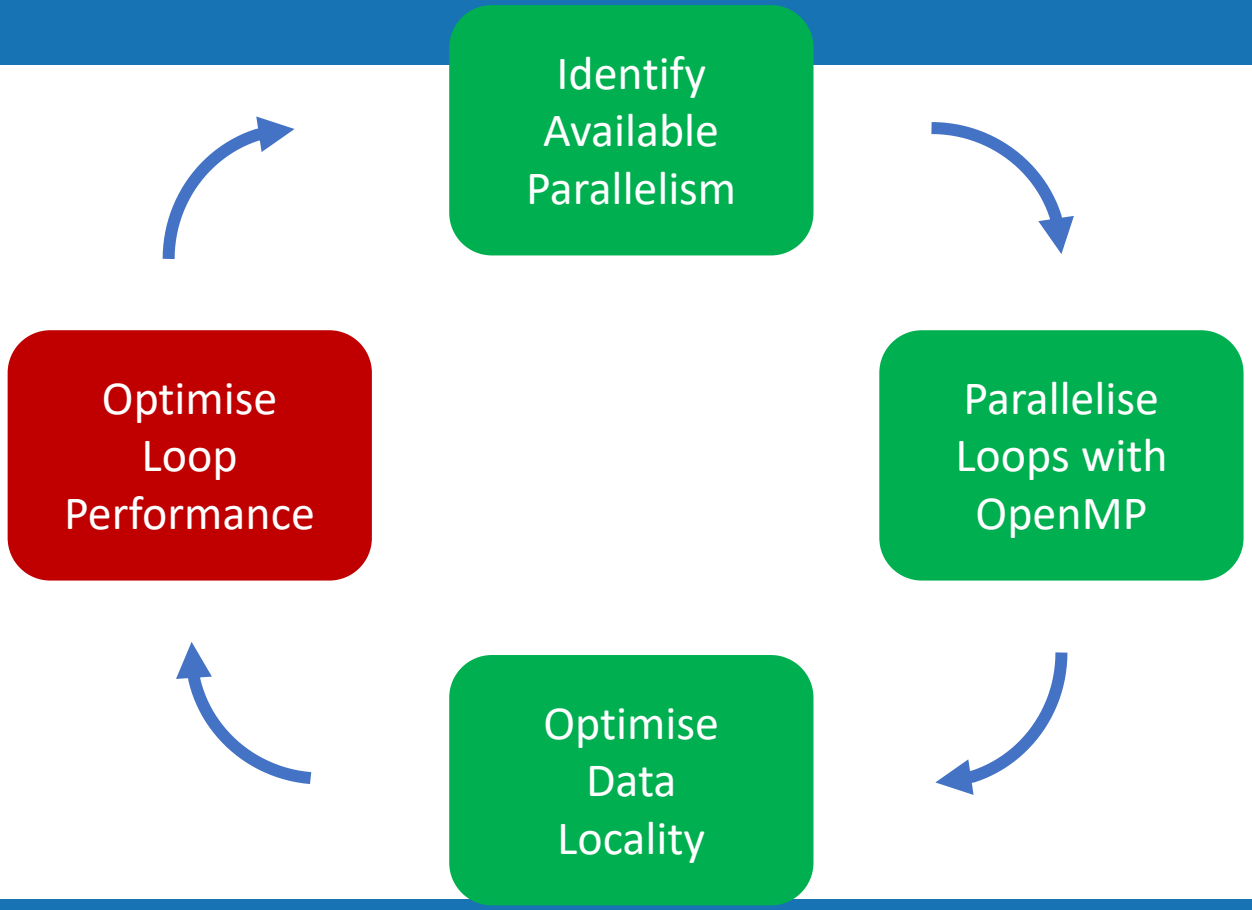


Copy A,Anew to/from the device


# Exercise: Performance

- Add the data region
- What is the performance improvement?
  - Try excluding the data movement operations!
  - Try running for more iterations (max_iters)
  - Try running with a larger mesh!
- What is reported when export CRAY_ACC_DEBUG=1?

- Calculate absolute performance metrics
  - Achieved bandwidth for the application
  - See how achieved bandwidth depends on e.g. problem size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# OpenMP `collapse` clause

- `collapse(n)` : Transform the following n tightly nested loops into one, flattened loop.
- Useful when individual loops lack sufficient parallelism or more than 3 loops are nested

```
#pragma omp target distribute parallel for collapse(2)
for(int i=0; i<N; i++)
for(int j=0; j<N; j++) ...
```

```
#pragma omp target distribute parallel for
for(int ij=0; ij<N*N; ij++)
...
```


# Exercise

- Open Lab 7 cg.cpp
- Parallelise with OpenMP CPU/GPU
  - Use collapse wisely!
  - Plenty of reductions
- Compare performance on CPU vs. GPU


# Homework – due Apr 21

- Add OpenMP GPU offload to our lbm_d2q9 project
  - Analogous to CPU side OpenMP
  - Use data regions