Programming your GPU with OpenMP

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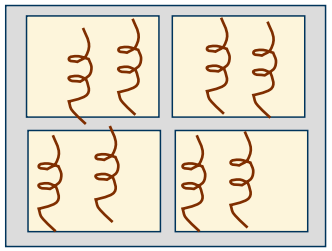
The Human Learning Group

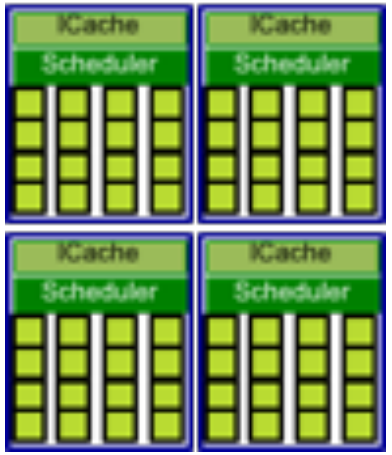
This content was created with Tom Deakin and Simon McIntosh-Smith of the University of Bristol

Hardware is diverse … and its only getting worse!!!

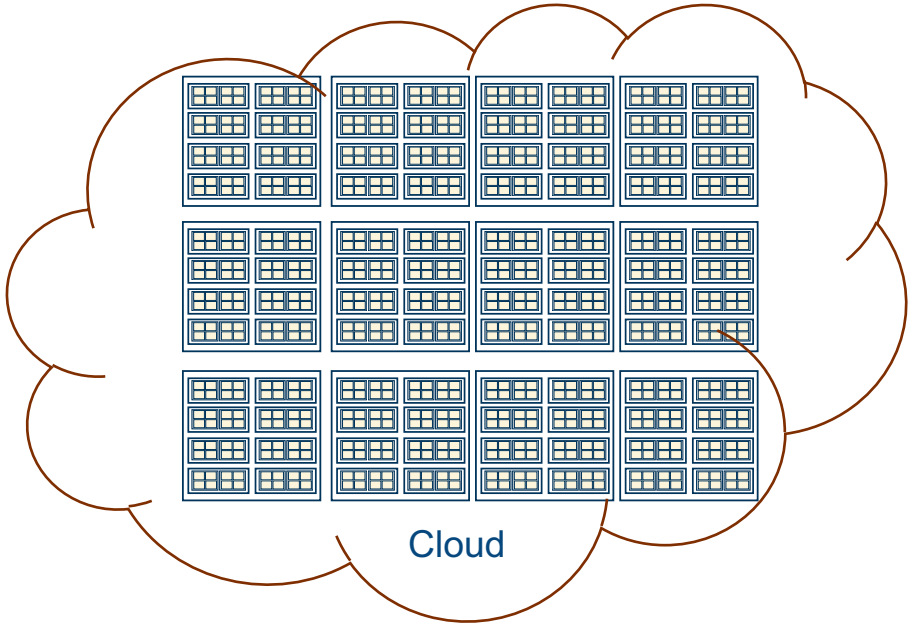


CPU

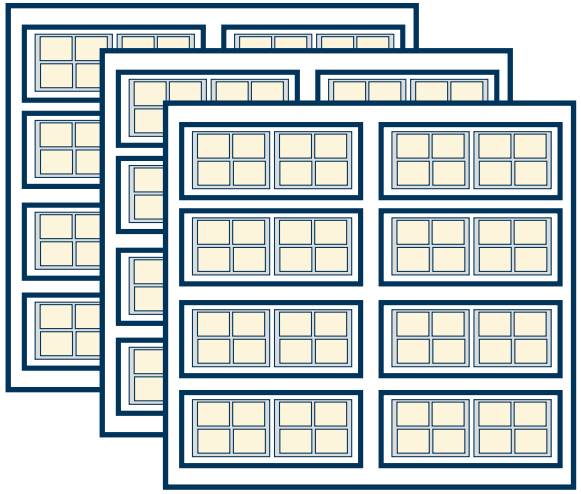
SIMD/Vector



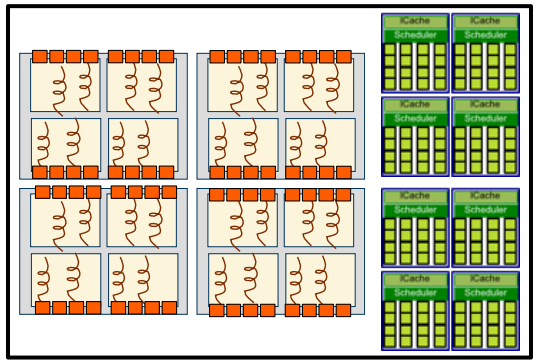
GPU



Cloud



Cluster



Heterogeneous node

The Big Three

You will know the basics of MPI

- In HPC, 3 programming environments dominate … covering the major classes of hardware.
  - **MPI**: distributed memory systems … though it works nicely on shared memory computers.
  - **OpenMP**: Shared memory systems … more recently, GPGPU too.
  - **CUDA**, **OpenCL**, **Sycl**, **OpenACC**, **OpenMP** … : GPU programming (use CUDA if you don't mind locking yourself to a single vendor … it is a really nice programming model)

You are all OpenMP experts and know a great deal about multithreading

- Even if you don't plan to spend much time programming with these systems … a well rounded HPC programmer should know what they are and how they work.

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The "new" kid on the block … GPUs

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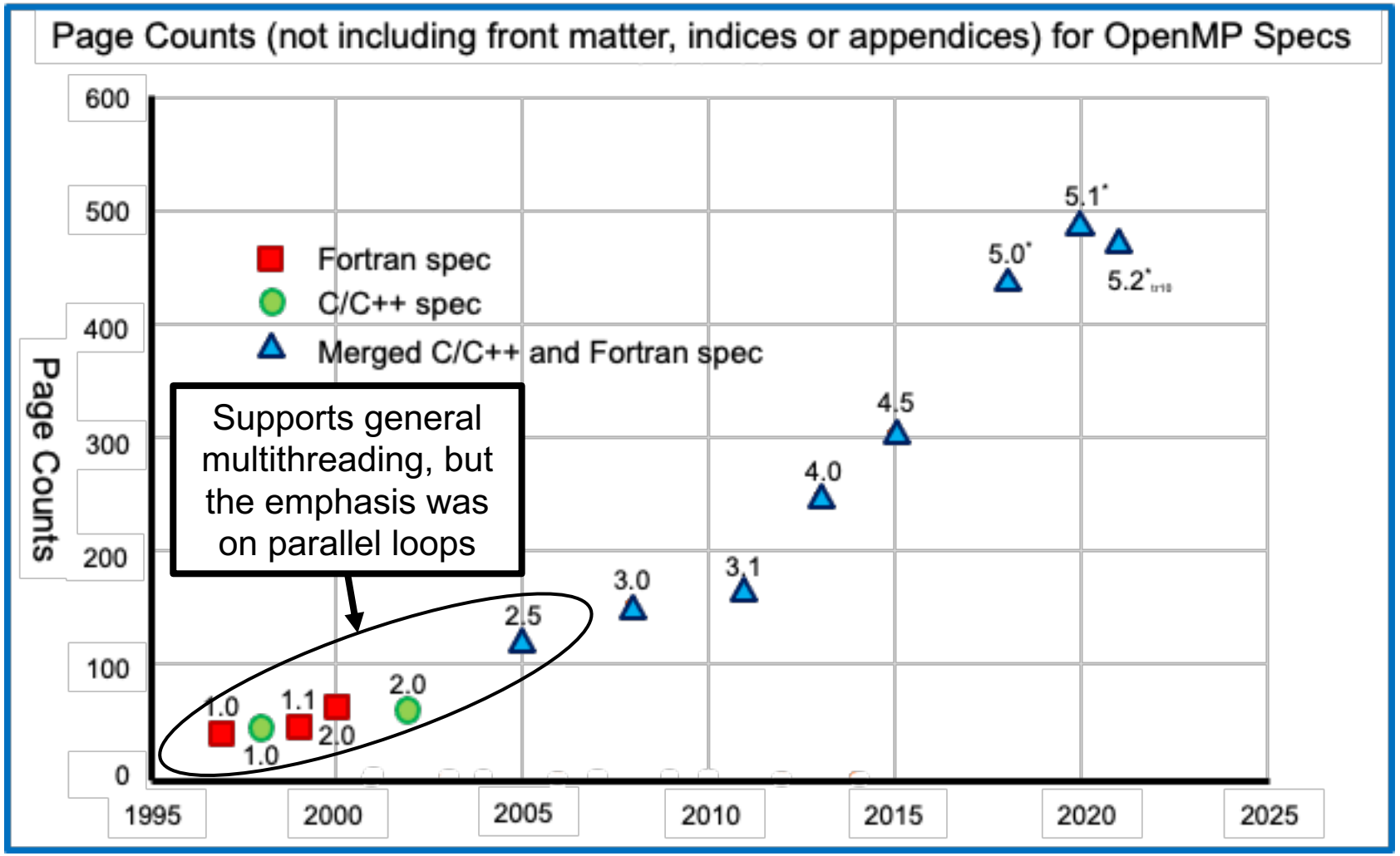
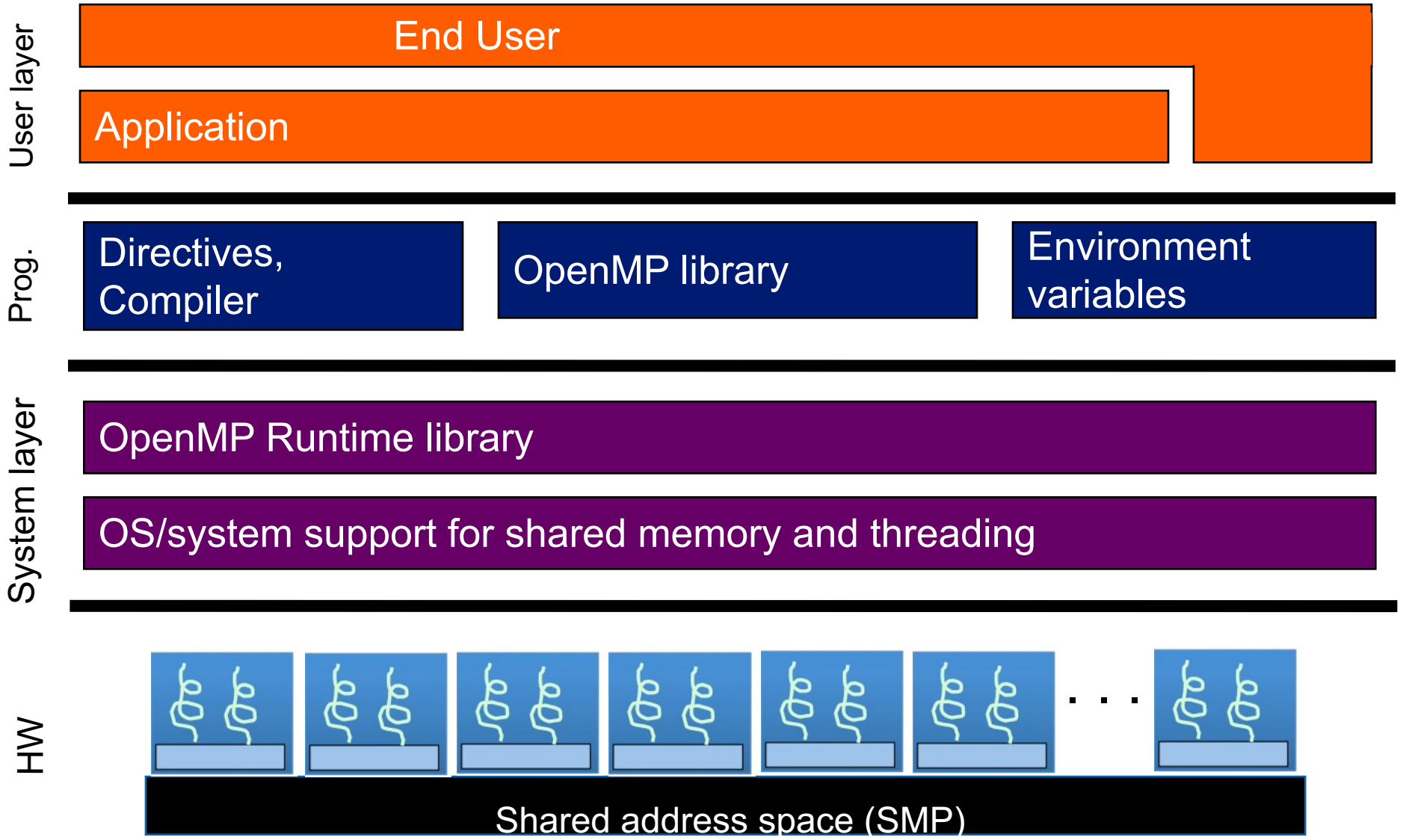
The growth of complexity in OpenMP

- OpenMP started out in 1997 as a simple interface for the application programmers more versed in their area of science than computer science.

- The complexity has grown considerably over the years!



OpenMP Basic Definitions: Basic Solution Stack



For the OpenMP Common Core, we focus on Symmetric Multiprocessor Case ….
i.e., lots of threads with “equal cost access” to memory

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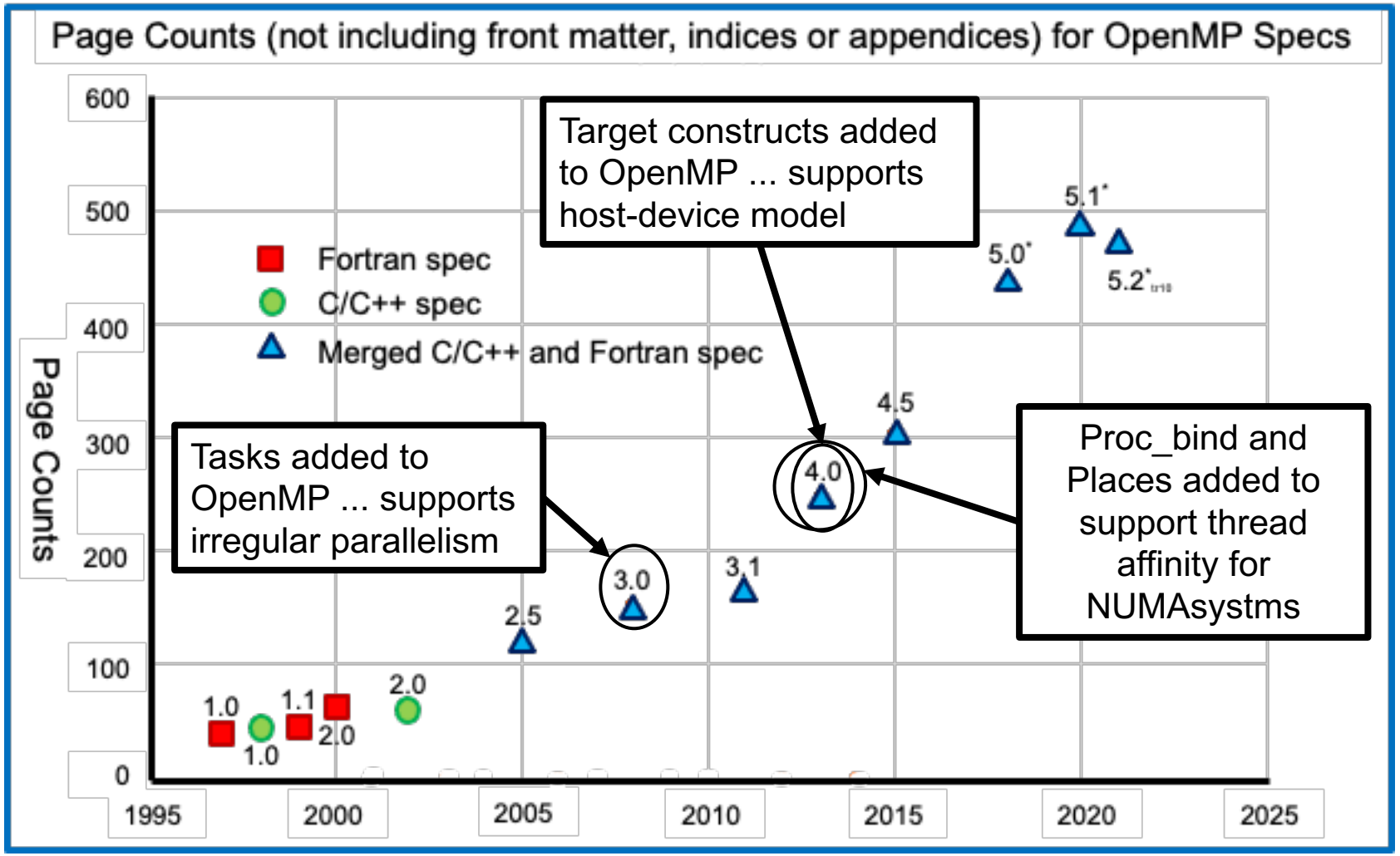

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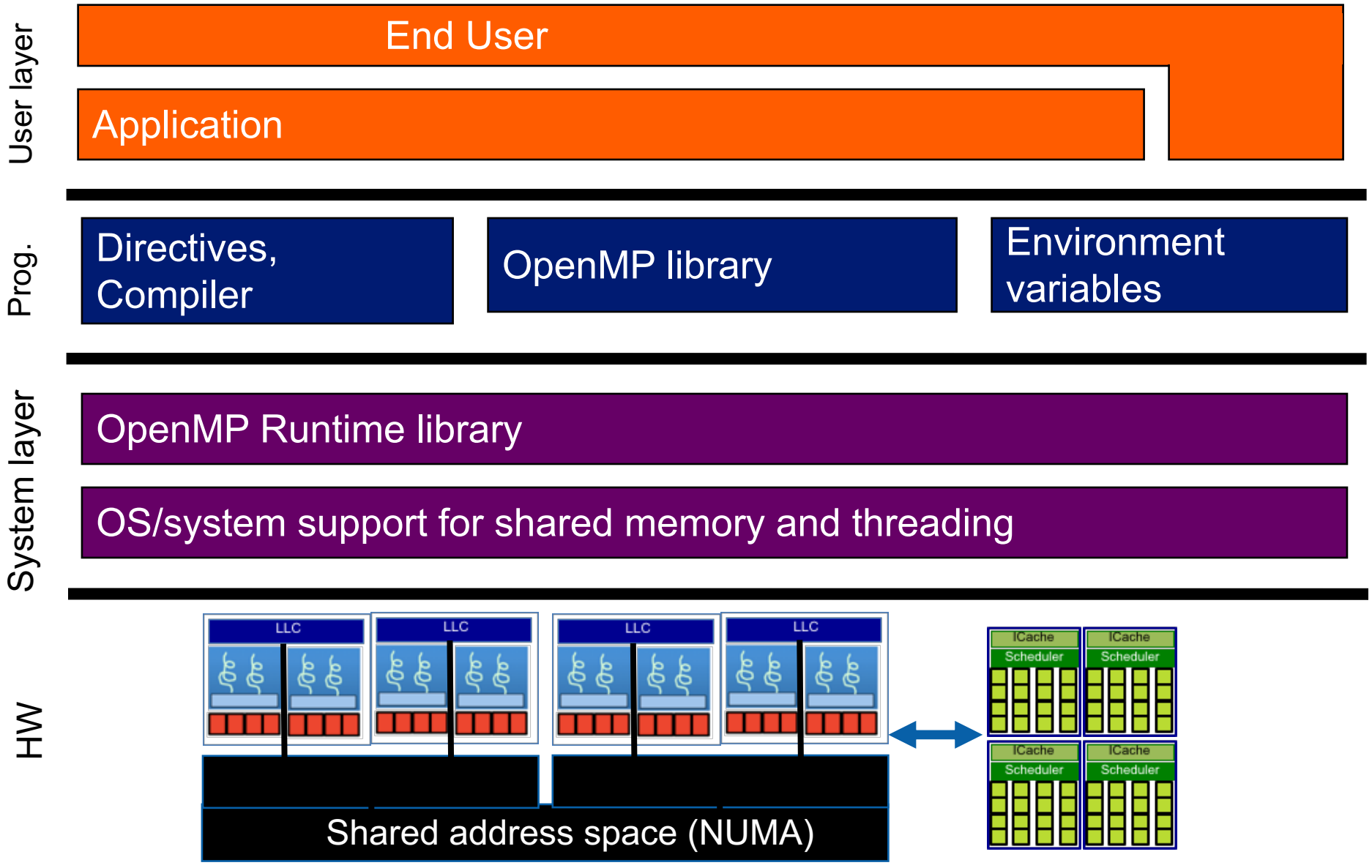


The "BIG idea" Behind GPU programming

Traditional Loop based vector addition (vadd)

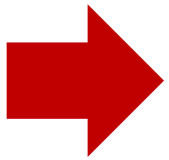
```
int main() {
   int N = . . . ;
   float *a, *b, *c;

   a* =(float *) malloc(N * sizeof(float));

   // ... allocate other arrays (b and c)
   // and fill with data

   for (int i=0;i<N; i++)
      c[i] = a[i] + b{i];

}
```



Data Parallel vadd with CUDA

```
// Compute sum of length-N vectors: C = A + B
void __global__
vecAdd (float* a, float* b, float* c, int N) {
    int i = blockIdx.x * blockDim.x + threadIdx.x;
    if (i < N) c[i] = a[i] + b[i];
}

int main () {
    int N = ... ;
    float *a, *b, *c;
    cudaMalloc (&a,  sizeof(float) * N);
  // ... allocate other arrays (b and c)
  // and fill with data

  // Use thread blocks with 256 threads each
    vecAdd <<< (N+255)/256, 256 >>> (a, b, c, N);
}
```

Assume a GPU with unified shared memory … allocate on host, visible on device too

How do we execute code on a GPU: The SIMT model (Single Instruction Multiple Thread)

1. Turn source code into a scalar work-item

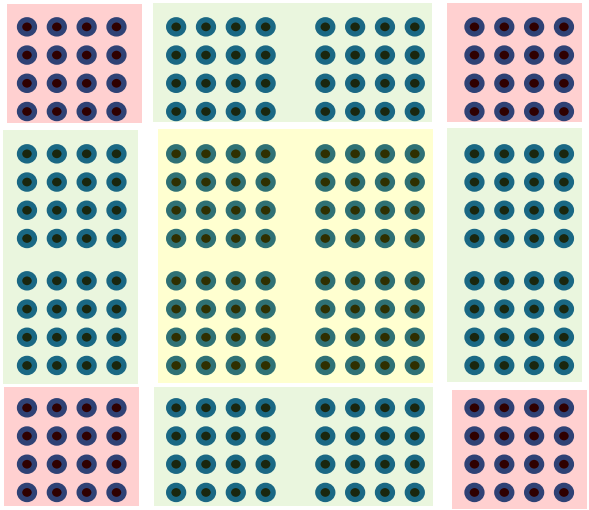
```
// Compute sum of length-N vectors: C = A + B
void __global__
vecAdd (float* a, float* b, float* c, int N)
{
    int i = blockIdx.x * blockDim.x +
threadIdx.x;
    if (i < N) c[i] = a[i] + b[i];
}

int main () {
    int N = ... ;
    float *a, *b, *c;
    cudaMalloc (&a,  sizeof(float) * N);
  // ... allocate other arrays (b and c)
  // and fill with data

  // Use thread blocks with 256 threads each
    vecAdd <<< (N+255)/256, 256 >>> (a, b, c,
N);
}
```

This is CUDA code … the sort of code the OpenMP compiler generates on your behalf

2. Map work-items onto an N dim index space.

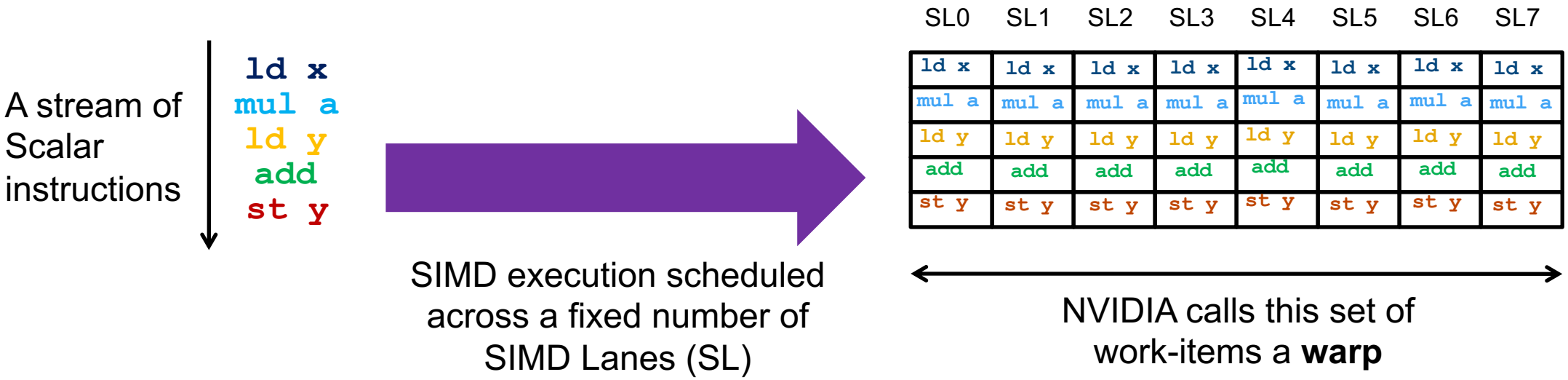


3. Map data structures onto the same index space

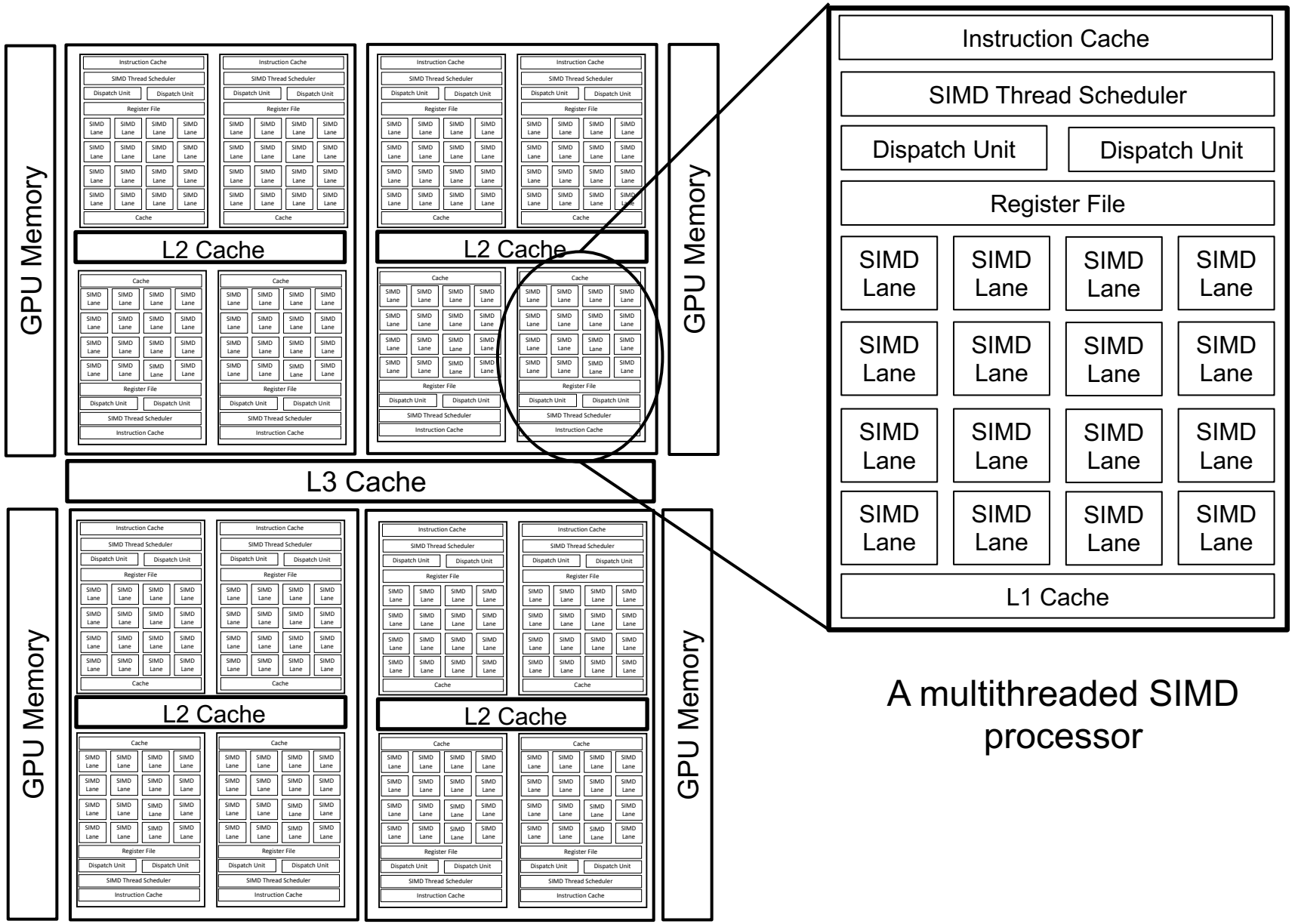
4. Run on hardware designed around the same SIMT execution model

SIMT: One instruction stream maps onto many SIMD lanes

- SIMT model: Individual scalar instruction streams are grouped together for SIMD execution on hardware

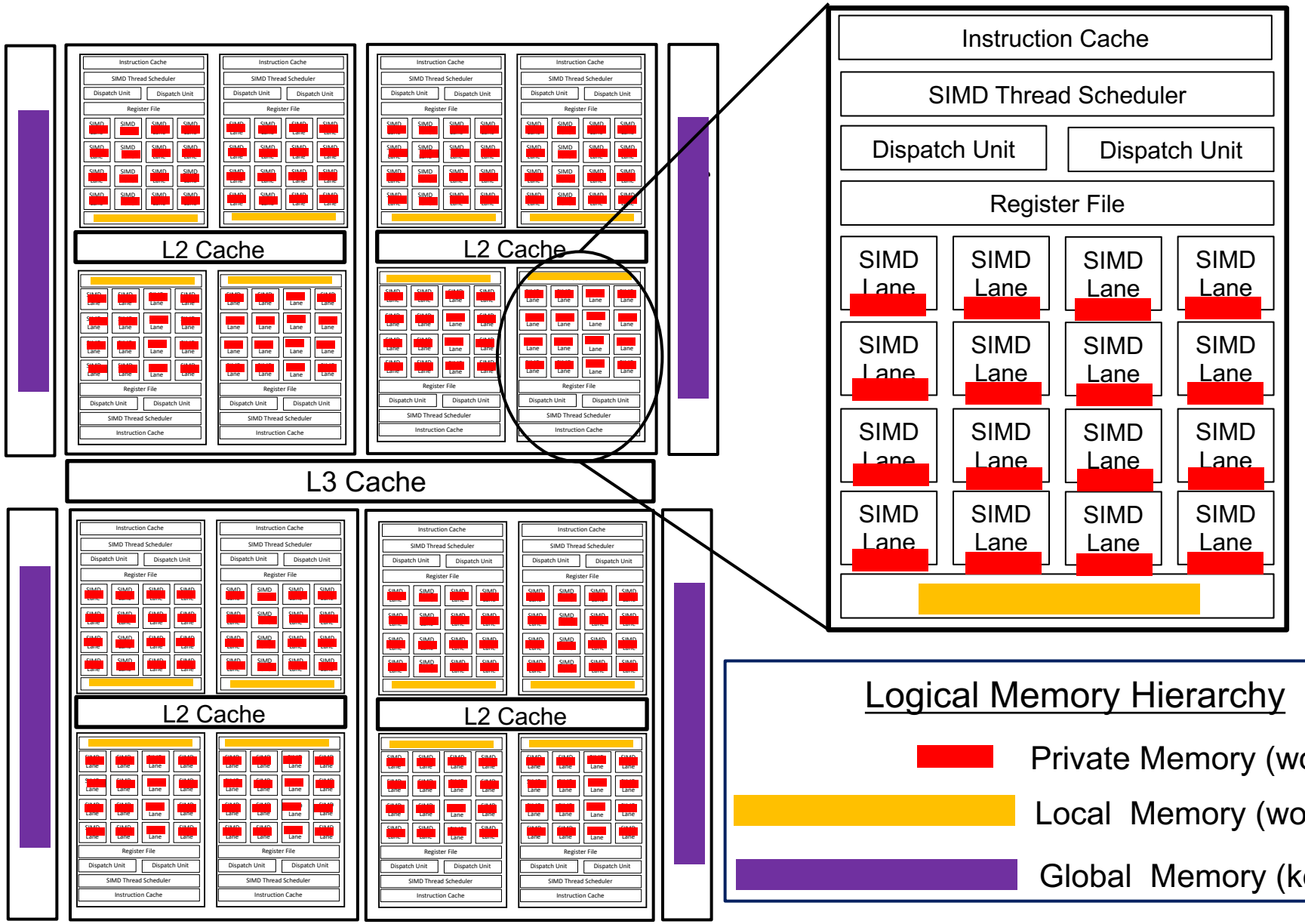


A Generic GPU (following Hennessey and Patterson)



A multithreaded SIMD processor

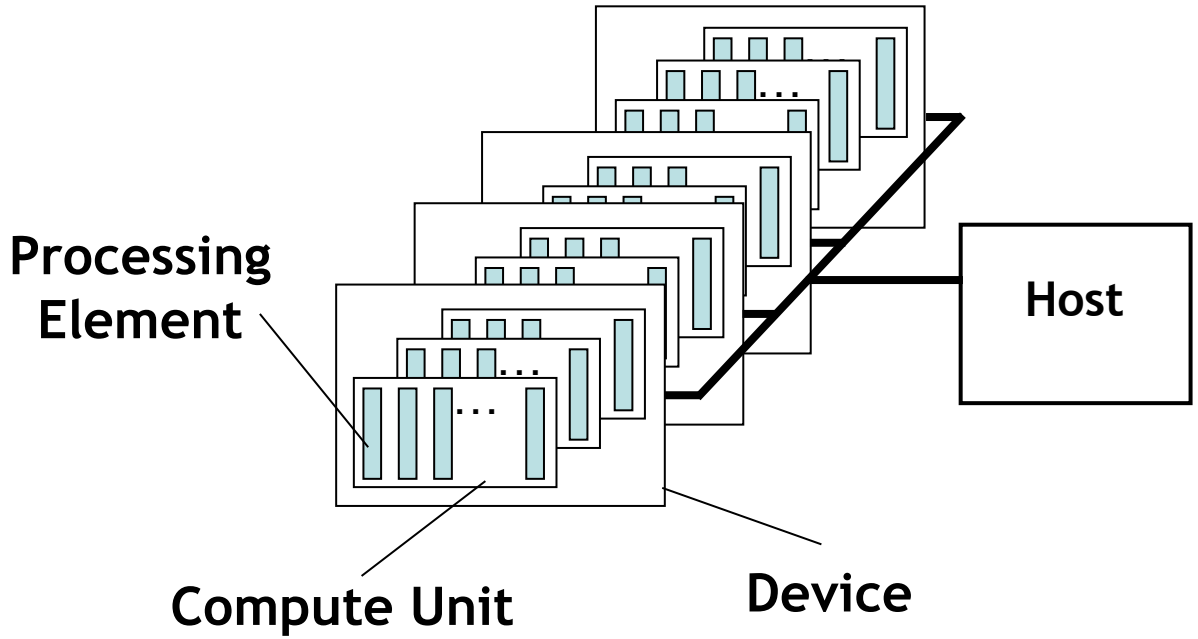
A Generic GPU (following Hennessey and Patterson)



GPU terminology is Broken (sorry about that)

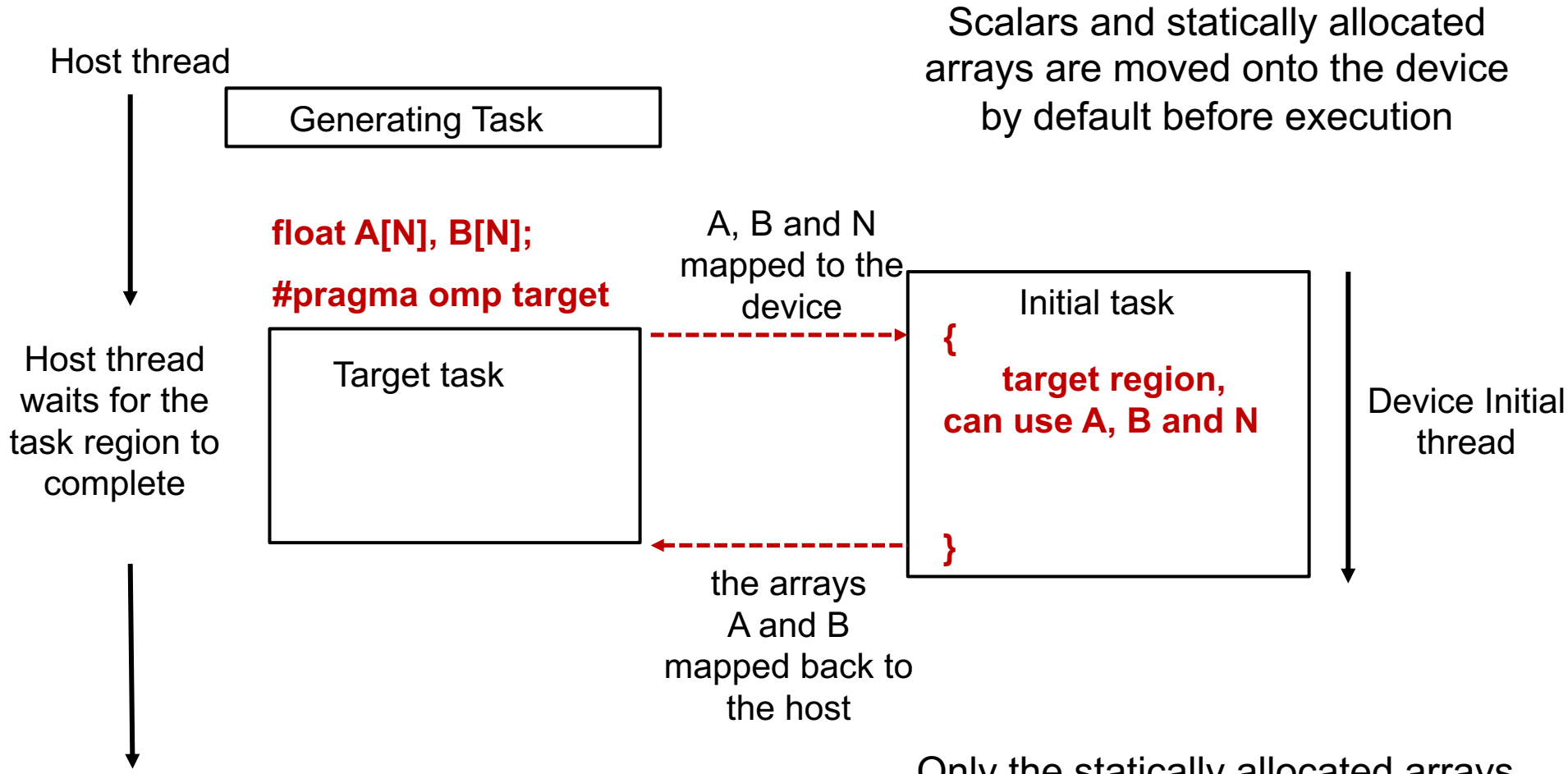
Hennessy and Patterson	CUDA	OpenCL
Multithreaded SIMD Processor	Streaming multiprocessor	Compute Unit
SIMD Thead Scheduler	Warp Scheduler	Work-group scheduler
SIMD Lane	CUDA Core	Processing Element
GPU Memory	Global Memory	Global Memory
Private Memory	Local Memory	Private Memory
Local Memory	Shared Memory	Local Memory
Vectorizable Loop	Grid	NDRange
Sequence of SIMD Lane operations	CUDA Thread	work-item
A thread of SIMD instructions	Warp	sub-group

A Generic Host/Device Platform Model



- One ***Host*** and one or more ***Devices***
  - Each Device is composed of one or more Compute Units
  - Each Compute Unit is divided into one or more ***Processing Elements***
- Memory divided into ***host memory*** and ***device memory***

Running code on the GPU:
The target construct and default data movement



Based on figure 6.4 in **Using OpenMP – The Next Step** by van der Pas, Stotzer and Terboven, MIT Press, 2017

Default Data Sharing: example

```
int main(void) {
  int N = 1024;
  double A[N], B[N];

  #pragma omp target
  {

    for (int ii = 0; ii < N; ++ii) {

      A[ii] = A[ii] + B[ii];

    }

  } // end of target region
}
```

1. Variables created in host memory.

2. Scalar **N** and stack arrays **A** and **B** are copied *to* device memory. Execution transferred to device.

3. **ii** is **private** on the device as it's declared within the target region

4. Execution on the device.

5. stack arrays **A** and **B** are copied *from* device memory back to the host. Host resumes execution.

Now let's run code in parallel on the device

```
int main(void) {
  int N = 1024;
  double A[N], B[N];

  #pragma omp target
  {
    #pragma omp loop
    for (int ii = 0; ii < N; ++ii) {

      A[ii] = A[ii] + B[ii];

    }

  } // end of target region
}
```

The loop construct tells the compiler:

"this loop will execute correctly if the loop iterations run in any order. You can safely run them concurrently. And the loop-body doesn't contain any OpenMP constructs. So do whatever you can to make the code run fast"

The loop construct is a declarative construct. You tell the compiler what you want done but you DO NOT tell it how to "do it". This is new for OpenMP

Exercise: Parallel vector addition on a GPU

- Make a copy of your parallel vadd.c program for a CPU (i.e. save the CPU version)
  - vadd.c Adds together two arrays, element by element: for(i=0;i<N;i++) c[i]=a[i]+b[i];
- Parallelize your vadd program for a GPU
- Time it for large N and save the result. How does it compare to the CPU version?
  - double omp_get_wtime();
  - #pragma omp target
  - #pragma omp loop

For tiny little programs, OpenMP may opt to run the code on the host. You can force the OpenMP runtime to use the GPU by setting the OMP_TARGET_OFFLOAD environment variable

> OMP_TARGET_OFFLOAD=MANDATORY ./a.out

Get interactive access to a node:

```
qsub -I -l select=1 -l walltime=00:30:00 -l filesystems=home:grand:eagle  -A ATPESC2024 -q R2035670
```

Compiler with cc … which is a wrapper around the Nvidia compilers (cc, CC or ftn)

```
cc -mp=gpu program.c
```

ParPorgForPhys/OMP_GPU_Exercises/vadd.c

Solution: Simple vector add in OpenMP on GPU

```
int main()
{
    float a[N], b[N], c[N], res[N];
    int err=0;

   // fill the arrays
   #pragma omp parallel for
   for (int i=0; i<N; i++){
      a[i] = (float)i;
      b[i] = 2.0*(float)i;
      c[i] = 0.0;
      res[i] = i + 2*i;
   }

   // add two vectors
   #pragma omp target
   #pragma omp loop
   for (int i=0; i<N; i++){
      c[i] = a[i] + b[i];
   }

   // test results
   #pragma omp parallel for reduction(+:err)
   for(int i=0;i<N;i++){
      float val = c[i] - res[i];
      val = val*val;
      if(val>TOL) err++;
   }
   printf("vectors added with %d errors\n", err);
   return 0;
}
```

CUDA Toolkit: nsys

Simple profiling: nsys nvprof ./*exe* <*params*>

```
> nsys nvprof ./flow.omp4. flow-params
Problem dimensions 4000x4000 for 1 iterations.
==188532== NVPROF is profiling process 188532, command: ./flow.omp4 flow.params
Number of ranks: 1
Number of threads: 1

Iteration 1
Timestep:         1.816932845523e-04
Total mass:       2.561400875000e+06
Total energy:     5.442884982081e+06
Simulation time: 0.0001s
Wallclock:        0.0325s

Expected energy  3.231871108096e+07, result was 3.231871108096e+07.
Expected density 2.561400875000e+06, result was 2.561400875000e+06.
PASSED validation.
Wallclock 0.0325s, Elapsed Simulation Time 0.0001s
==188532== Profiling application: ./flow.omp4 flow.params
==188532== Profiling result:
Time(%)      Time     Calls       Avg       Min       Max  Name
 55.51%  205.74ms        53  3.8818ms     896ns  12.821ms  [CUDA memcpy HtoD]
 28.69%  106.32ms        14  7.5942ms     576ns  55.648ms  [CUDA memcpy DtoH]
  5.31%  19.682ms         2  9.8411ms  3.8686ms  15.814ms  set_problem_2d$ck_L240_28
  1.52%  5.6321ms         2  2.8160ms  2.8121ms  2.8199ms  set_timestep$ck_L92_5
  1.05%  3.9072ms        32  122.10us  1.2160us  217.21us  allocate_data$ck_L30_1
  0.80%  2.9801ms         1  2.9801ms  2.9801ms  2.9801ms  artificial_viscosity$ck_L198_16
  0.73%  2.7061ms         1  2.7061ms  2.7061ms  2.7061ms  pressure_acceleration$ck_L128_9
```

Time to copy data onto GPU

Time to copy data back from GPU

Exercise: Parallel vector addition on a GPU

- Run you vector add program using nsys and see if the profiling output matches your expectations for vadd.
  - double omp_get_wtime();
  - #pragma omp parallel
  - #pragma omp for
  - #pragma omp parallel for
  - #pragma omp task
  - #pragma omp taskwait
  - #pragma single
  - #pragma omp target
  - #pragma omp loop

For tiny little programs, OpenMP may opt to run the code on the host. You can force the OpenMP runtime to use the GPU by setting the OMP_TARGET_OFFLOAD environment variable

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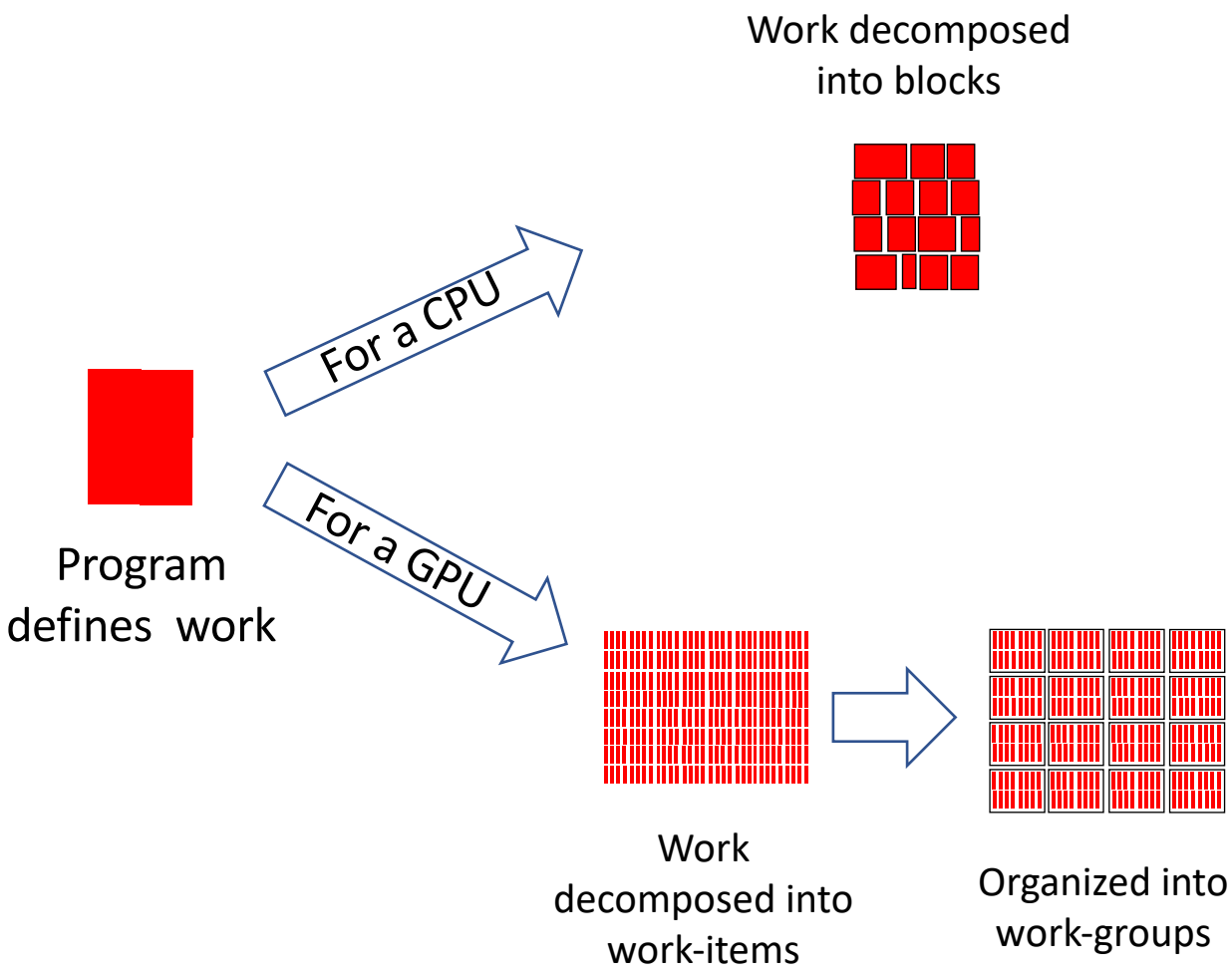
Compiler with cc … which is a wrapper around the Nvidia compilers (cc, CC or ftn)

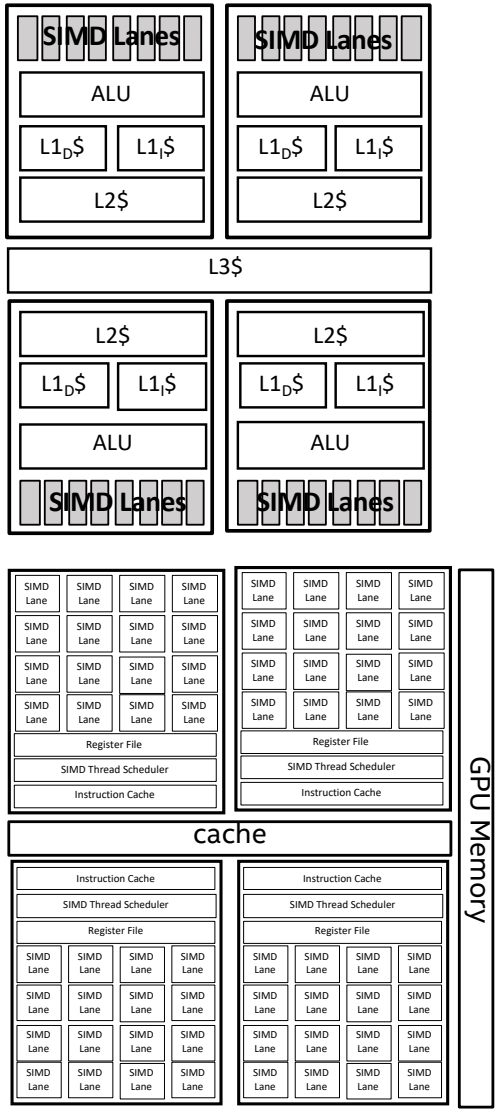
```
cc -mp=gpu program.c
nsys nvprof ./a.out
```

ParPorgForPhys /OMP_GPU_Exercises/vadd.c

Let’s compare/contrast concurrency on a CPU and a GPU

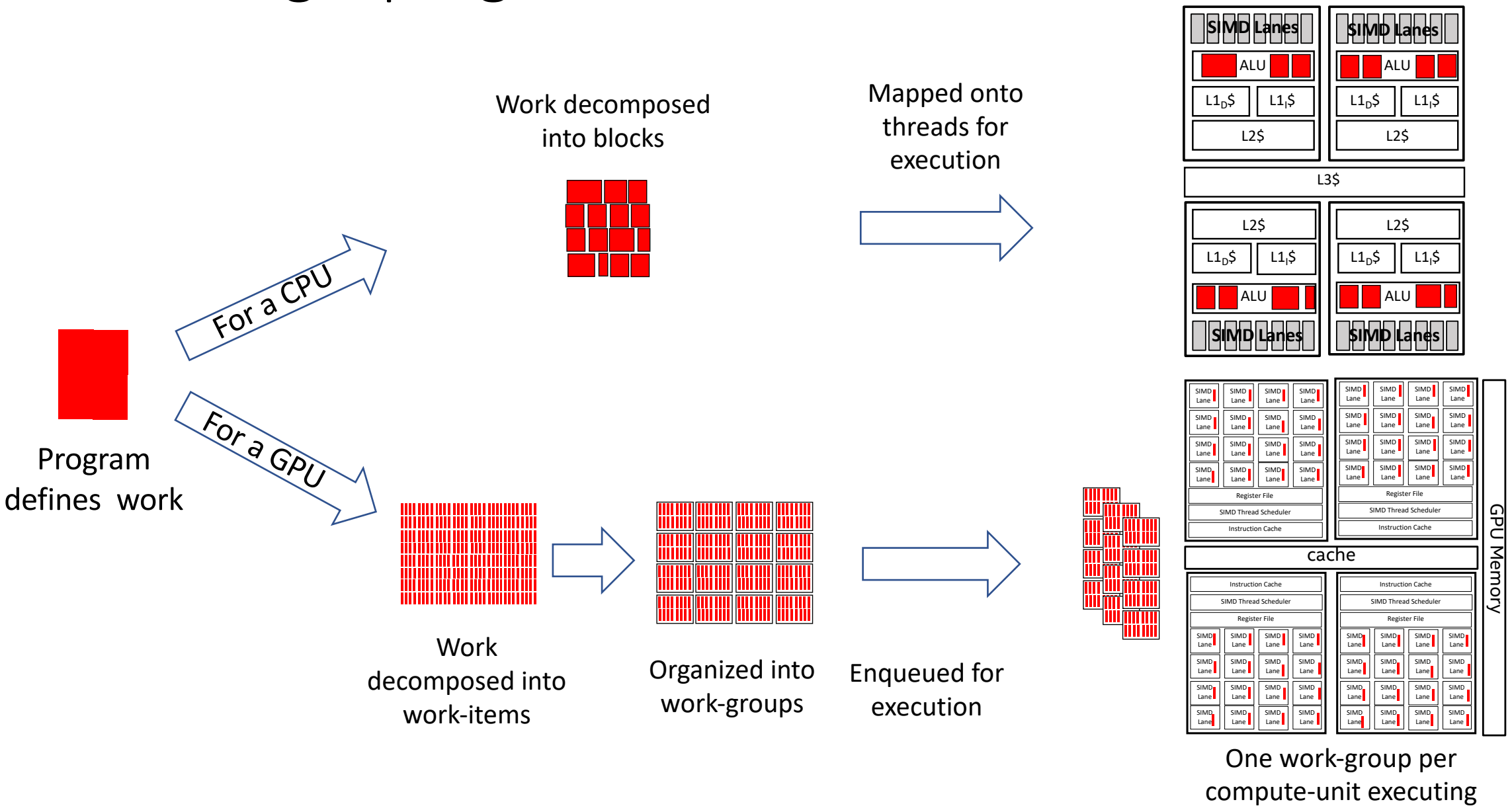
Executing a program on CPUs and GPUs



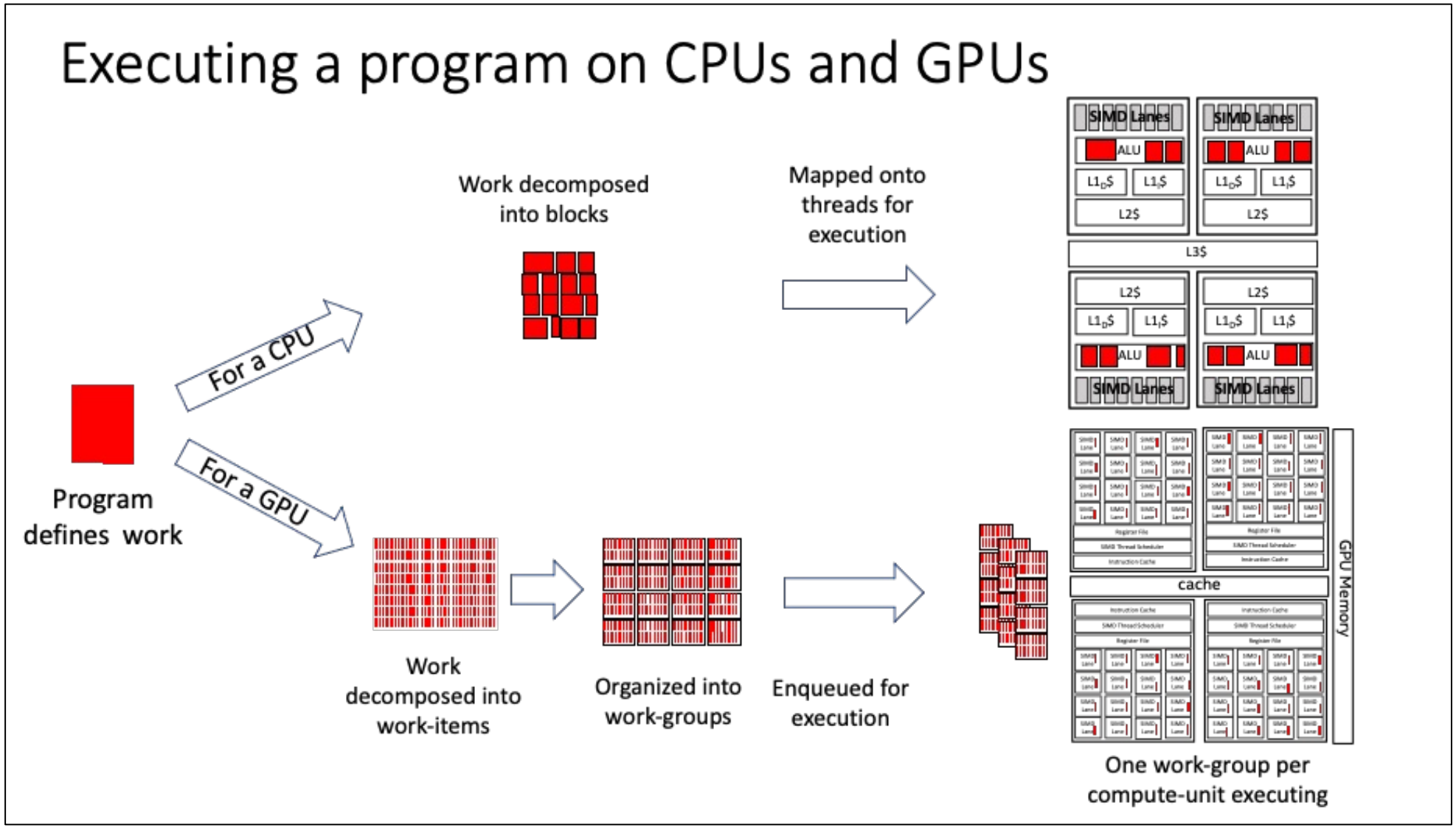


One work-group per compute-unit executing

Executing a program on CPUs and GPUs



CPU/GPU execution modesl



For a CPU, the threads are all active and able to make forward progress.

For a GPU, any given work-group might be in the queue waiting to execute.

Implicit data movement covers a small subset of the cases you need in a real program.

To be more general … we need to manage data movement explicitly

Explicit data movement

- Previously, we described the rules for *implicit* data movement.
- We can *explicitly* control the movement of data using the **map** clause.
- **Data allocated on the heap needs to be explicitly copied to/from the device**:

```
int main(void) {
   int  ii=0, N = 1024;
   int* A = (int *)malloc(sizeof(int)*N);

   #pragma omp target
   {
     // N, ii and A all exist here
     // The data that A points to (*A , A[ii]) DOES NOT exist here!
   }
}
```

Moving data with the map clause

```
int main(void) {
   int  N = 1024;
   int* A = malloc(sizeof(int)*N);

   #pragma omp target map(A[0:N])
   {
     // N, ii and A all exist here
     // The data that A points to DOES exist here!
   }
}
```

Default mapping
map(tofrom: A[0:N])

Copy at start and end of **target** region.

OpenMP array notation

- For mapping data arrays/pointers you must use array section notation:
  - In C, notation is **pointer[lower-bound : length]**
  - **map(to: a[0:N])**
  - Starting from the element at a[0], copy N elements to the target data region
  - **Be careful!**
    - It's common to confuse this with the Fortran notation: (begin : end).
  - Without the map, OpenMP defines that the pointer itself (**a**) is mapped as a zero-length array section.
    - Zero length arrays: a[:0]

Controlling data movement

```
int i, a[N], b[N], c[N];
#pragma omp target map(to:a,b) map(tofrom:c)
```

Data movement defined from the *host* perspective.

- The various forms of the map clause
  - **map(to:list)**: On entering the region, variables in the list are initialized on the device using the original values from the host (host to device copy).
  - **map(from:list)**: At the end of the target region, the values from variables in the list are copied into the original variables on the host (device to host copy). On entering the region, the initial value of the variables on the device is not initialized.
  - **map(tofrom:list)**: the effect of both a map-to and a map-from (host to device copy at start of region, device to host copy at end).
  - **map(alloc:list)**: On entering the region, data is allocated and uninitialized on the device.
  - **map(list)**: equivalent to **map(tofrom:list)**.

Exercise: Parallel vector addition on a GPU

- Start from vadd_heap.c
  - Vadd_heap.c Adds together two arrays, element by element: for(i=0;i<N;i++) c[i]=a[i]+b[i];
- Parallelize for a GPU
  - double omp_get_wtime();
  - #pragma omp parallel
  - #pragma omp for
  - #pragma omp parallel for
  - #pragma omp task
  - #pragma omp taskwait
  - #pragma single
  - #pragma omp target
  - #pragma omp loop
  - Plus the clauses
    - private(), firstprivate(), reduction(+:var)
    - map(to:vptr[Lower:Count]) map(from:vptr[Lower:Count]) map(tofrom:vptr[Lower:Count])

Default is tofrom: map(vptr[Lower:Count])

ParPorgForPhys /OMP_GPU_Exercises/vadd.c

Solution: vector add with dynamic memory on GPU

```
int main()
{
    float *a   = malloc(sizeof(float) * N);
    float *b   = malloc(sizeof(float) * N);
    float *c   = malloc(sizeof(float) * N);
    float *res = malloc(sizeof(float) * N);
    int err=0;

   // fill the arrays <<<code not shown>>>>

   // add two vectors
   #pragma omp target map(to: a[0:N],b[0:N]) map (tofrom: c[0:N])
   #pragma omp loop
   for (int i=0; i<N; i++){
      c[i] = a[i] + b[i];
   }

  // test results <<<code not shown>>>>

  #pragma omp parallel for reduction(+:err)
  printf("vectors added with %d errors\n", err);
  return 0;
}
```

Commonly used clauses on target and loop constructs

- The basic construct* is:

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

  #pragma omp loop *[clause[[,]clause]...]*

  for-loops

- The most commonly used clauses are:
  - **map(to | from | tofrom list)** ← default is tofrom
  - **private(***list***)** **firstprivate(***list***)** **lastprivate(***list***)** **shared(***list***)**
    - behave as data environment clauses in the rest of OpenMP, but note values are only created or copied into the region, not back out “at the end”.
  - **reduction(***reduction-identifier* **:** *list***)**
    - behaves as in the rest of OpenMP
  - **collapse(***n***)**
    - Combines loops before the distribute directive splits up the iterations between teams

Going beyond simple vector addition …

Using OpenMP for GPU application programming … the heat diffusion problem

5-point stencil: the heat program

- The heat equation models changes in temperature over time.

$$\frac{\partial u}{\partial t} - \alpha \nabla^2 u = 0$$

- We'll solve this numerically on a computer using an explicit **finite difference** discretisation.
- $u = u(t, x, y)$ is a function of space and time.
- Partial differentials are approximated using diamond difference formulae:

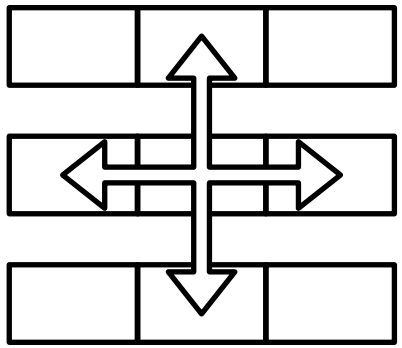
$$\frac{\partial u}{\partial t} \approx \frac{u(t+1, x, y) - u(t, x, y)}{dt}$$

$$\frac{\partial^2 u}{\partial x^2} \approx \frac{u(t, x+1, y) - 2u(t, x, y) + u(t, x-1, y)}{dx^2}$$

  - Forward finite difference in time, central finite difference in space.

5-point stencil: the heat program

- Given an initial value of u, and any boundary conditions, we can calculate the value of u at time t+1 given the value at time t.
- Each update requires values from the north, south, east and west neighbours only:



- Computation is essentially a weighted average of each cell and its neighbouring cells.
- If on a boundary, look up a boundary condition instead.

Method of Manufactured Solution

- Stencil codes are notoriously difficult to **know** if the answer is “correct”.

- Analytic solutions hard to come by:
  - It’s why you’re using a computer to solve the equation approximately after all!

- Method of Manufactured Solution (MMS) is a way to help determine if the code does the correct thing.
- An approach often used to find errors in CFD codes and check convergence properties.

Method of Manufactured Solution

- **Choose** a function for $u(t, x, y)$, substitute into the equation and work through the algebra.

- Ideally like the equation to evaluate to zero so don't need to consider a right-hand side to the equation.

- $u(0, x, y)$ gives the initial conditions.
- Can evaluate boundary conditions, e.g. bottom boundary $u(0,0, y)$

- Because u is **known** for all timesteps (it was chosen!), the exact solution is **known**.

- Compare the **computed** solution to the known u to compute an error.
- Any differences come from approximations in the method, or a bug in your code.

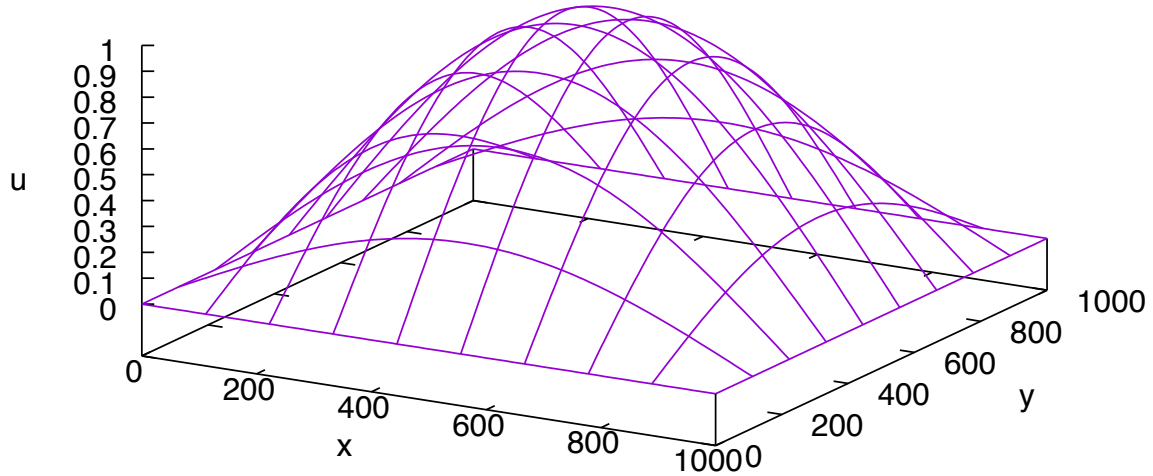
Method of Manufactured Solution

- For the problem of length l, choose u:

$$u(t,x,y) = e^{\frac{-2\alpha\pi^2 t}{l^2}} \sin\frac{\pi x}{l} \sin\frac{\pi y}{l}$$

- Boundary conditions: u is always zero on the boundaries

- Initial value of grid is then $u(0,x,y) = \sin\frac{\pi x}{l} \sin\frac{\pi y}{l}$



Heat program …

```
// Loop over time steps
for (int t = 0; t < nsteps; ++t) {

  // solve over spatial domain for step t
  solve(n, alpha, dx, dt, u, u_tmp);

  // Pointer swap to get ready for next step
  tmp = u;
  u = u_tmp;
  u_tmp = tmp;
}
```

- Takes two optional command line arguments: <ncells> <nsteps>
  - E.g. ./heat 1000 10
  - 1000x1000 cells, 10 timesteps (the default problem size).
- If no command line arguments are provided, it uses a default:
  - These two commands both run the default problem size of 1000x1000 cells, 10 timesteps.
  - ./heat
  - ./heat 1000 10
- A sensible bigger problem is 8000 x 8000 cells and 10 timesteps.

5-point stencil: solve kernel

```
void solve(…) {
  // Finite difference constant multiplier
  const double r = alpha * dt / (dx * dx);
  const double r2 = 1.0 - 4.0*r;

  // Loop over the nxn grid
  for (int i = 0; i < n; ++i) {
    for (int j = 0; j < n; ++j) {

      // Update the 5-point stencil, using boundary conditions on the edges of the domain.
      // Boundaries are zero because the MMS solution is zero there.
      u_tmp[i+j*n] =  r2 * u[i+j*n]           +
       r * ((i < n-1) ? u[i+1+j*n]   : 0.0) +
       r * ((i > 0)   ? u[i-1+j*n]   : 0.0) +
       r * ((j < n-1) ? u[i+(j+1)*n] : 0.0) +
       r * ((j > 0)   ? u[i+(j-1)*n] : 0.0);
    }
  }
}
```

Exercise: parallel stencil (heat)

- Take the provided heat stencil code (heat.c)
- Add OpenMP directives to parallelize the loops on the GPU
- Most of the runtime occurs in the solve() routine. Focus on that function. The rest of the code is there to just support the work inside solve.

  - double omp_get_wtime();
  - #pragma omp parallel
  - #pragma omp for
  - #pragma omp parallel for
  - #pragma omp task
  - #pragma omp taskwait
  - #pragma single
  - #pragma omp target
  - #pragma omp loop
  - Plus the clauses
    - private(), firstprivate(), reduction(+:var), collapse(n)
    - map(to:vptr[Lower:Count]) map(from:vptr[Lower:Count]) map(tofrom:vptr[Lower:Count])

After you get your program to work, profile it using nsys

Default is tofrom: map(vptr[Lower:Count])

Solution: parallel stencil (heat)

```
// Compute the next timestep, given the current timestep
void solve(const int n, const double alpha, const double dx, const double dt, const double * restrict u,
double * restrict u_tmp) {
  // Finite difference constant multiplier
  const double r = alpha * dt / (dx * dx);
  const double r2 = 1.0 - 4.0*r;

  // Loop over the nxn grid
  #pragma omp target map(tofrom: u[0:n*n], u_tmp[0:n*n])
  #pragma omp loop
  for (int i = 0; i < n; ++i) {
    for (int j = 0; j < n; ++j) {


      // Update the 5-point stencil, using boundary conditions on the edges of the domain.
      // Boundaries are zero because the MMS solution is zero there.
      u_tmp[i+j*n] =  r2 * u[i+j*n] +
      r * ((i < n-1) ? u[i+1+j*n] : 0.0) +
      r * ((i > 0)   ? u[i-1+j*n] : 0.0) +
      r * ((j < n-1) ? u[i+(j+1)*n] : 0.0) +
      r * ((j > 0)   ? u[i+(j-1)*n] : 0.0);
}}}
```

Data movement dominates!

```
for (int t = 0; t < nsteps; ++t) {
```

Typically lots of iterations!

```
  // Call the solve kernel
  // Computes u_tmp at the next timestep
  // given the value of u at the current timestep
  solve(n, alpha, dx, dt, u, u_tmp);

   // Pointer swap
   tmp = u;
   u = u_tmp;
   u_tmp = tmp;
}
```

For each iteration, copy to device $(2*N^2)*sizeof(TYPE)$ bytes

solve() routine uses this pragma:
#pragma omp target map(u_tmp[0:n*n], u[0:n*n])

For each iteration, copy from device $(2*N^2)*sizeof(TYPE)$ bytes

Finer control over data movement

- Recall that data is mapped to/from device at start/end of target region
  - #pragma omp target map(tofrom: A[0:N])
    {
      …
    }

- Inefficient to move data around all the time
- Want to keep data resident on the device *between* target regions
- Will explain how to interact with the device data environment

Target data directive

- The **target data** construct creates a target data region
  … use **map** clauses for explicit data management

Data is mapped onto the device at the beginning of the construct

```
#pragma omp target data map(to:A[0:N], B[0:M]) map(from: C[0:P])
{
    #pragma omp target
        {do lots of stuff with A, B and C}

    {do something on the host}

    #pragma omp target
        {do lots of stuff with A, B, and C}
}
```

one or more **target regions** work within the **target data region**

Data is mapped back to the host at the end of the target data region

Target update details

- **#pragma omp target update clause[[[,]clause]...]**
- Creates a target task to handle data movement between the host and a device.

- Clause: a motion-clause:
  - to(list)
  - from(list)

Target update directive

- You can update data between target regions with the **target update** directive.

Set up the data region ahead of time.

```
#pragma omp target data map(to: A[0:N],B[0:M]) map(from: C[0:P])
{
    #pragma omp target
        {do lots of stuff with A, B and C on the device}

    #pragma omp target update from(A[0:N])

    host_do_something_with(A)

    #pragma omp target update to(A[0:N])

    #pragma omp target
        {do lots more stuff with A, B, and C on the device}
}
```

map A on the device to A on the host.

map A on the host to A on the device.

Note: update directive has the transfer direction as the clause: e.g. update to(…)
Compare to map clause with direction inside: map(to: …)

Target enter/exit data constructs

- The **target data** construct requires a *structured* block of code.
  - Often inconvenient in real codes.

- Can achieve similar behavior with two standalone directives:
  #pragma omp target enter data map(…)
  #pragma omp target exit data map(…)

- The **target enter data** maps variables to the device data environment.
- The **target exit data** unmaps variables from the device data environment.
- Future **target** regions inherit the existing data environment.

Target enter/exit data example

```
void init_array(int *A, int N) {
   for (int i = 0; i < N; ++i)
      A[i] = i;
  #pragma omp target enter data map(to: A[0:N])
}

int main(void) {

   int N = 1024;
   int *A = malloc(sizeof(int) * N);
   init_array(A, N);

   #pragma omp target
   #pragma loop
   for (int i = 0; i < N; ++i)
      A[i] = A[i] * A[i];

 #pragma omp target exit data map(from: A[0:N])
}
```

Target enter/exit data details

- **#pragma omp target enter data clause[[[,]clause]...]**
- Creates a target task to handle data movement between the host and a device.

- clause is one of the following:
  - if(scalar-expression)
  - device(integer-expression)
  - map (map-type: list)

Exercise

- Modify your parallel heat code from the last exercise.
- Use the ‘target data’ family of constructs to control the device data environment.
- Minimize data movement with map clauses to minimize data movement.
- Question … will the pointer swap on the host still work?

  - #pragma omp target
  - #pragma omp target enter data
  - #pragma omp target exit data
  - #pragma omp target update
  - map(to:list) map(from:list) map(tofrom:list)
  - #pragma omp teams distribute parallel for simd

Solution: Pointer swapping in action

```
#pragma omp target enter data map(to: u[0:n*n], u_tmp[0:n*n])

 for (int t = 0; t < nsteps; ++t) {

    solve(n, alpha, dx, dt, u, u_tmp);

    // Pointer swap
    tmp = u;
    u = u_tmp;
    u_tmp = tmp;
  }

#pragma omp target exit data map(from: u[0:n*n])
```

Copy data to device before iteration loop

Update solve() routine to remove map clauses:
#pragma omp target ~~map(u_tmp[0:n*n], u[0:n*n])~~

Pointer-swap on the host works. Why?
The pointers (u and u_tmp) are "on the stack" scalars the value of which is a pointer to memory. They are copied onto the device at the target construct.
The association between host and device addresses is fixed with the start of a target data region. Hence, as you swap the pointers, the references to the addresses in device memory are swapped ….. i.e. pointer-swapping on the host works.

Copy data from device after iteration loop

Data movement summary

- Data transfers between host/device occur at:
  - Beginning and end of **target** region
  - Beginning and end of **target data** region
  - At the **target enter data** construct
  - At the **target exit data** construct
  - At the **target update** construct

- Can use **target data** and **target enter/exit data** to reduce redundant transfers.

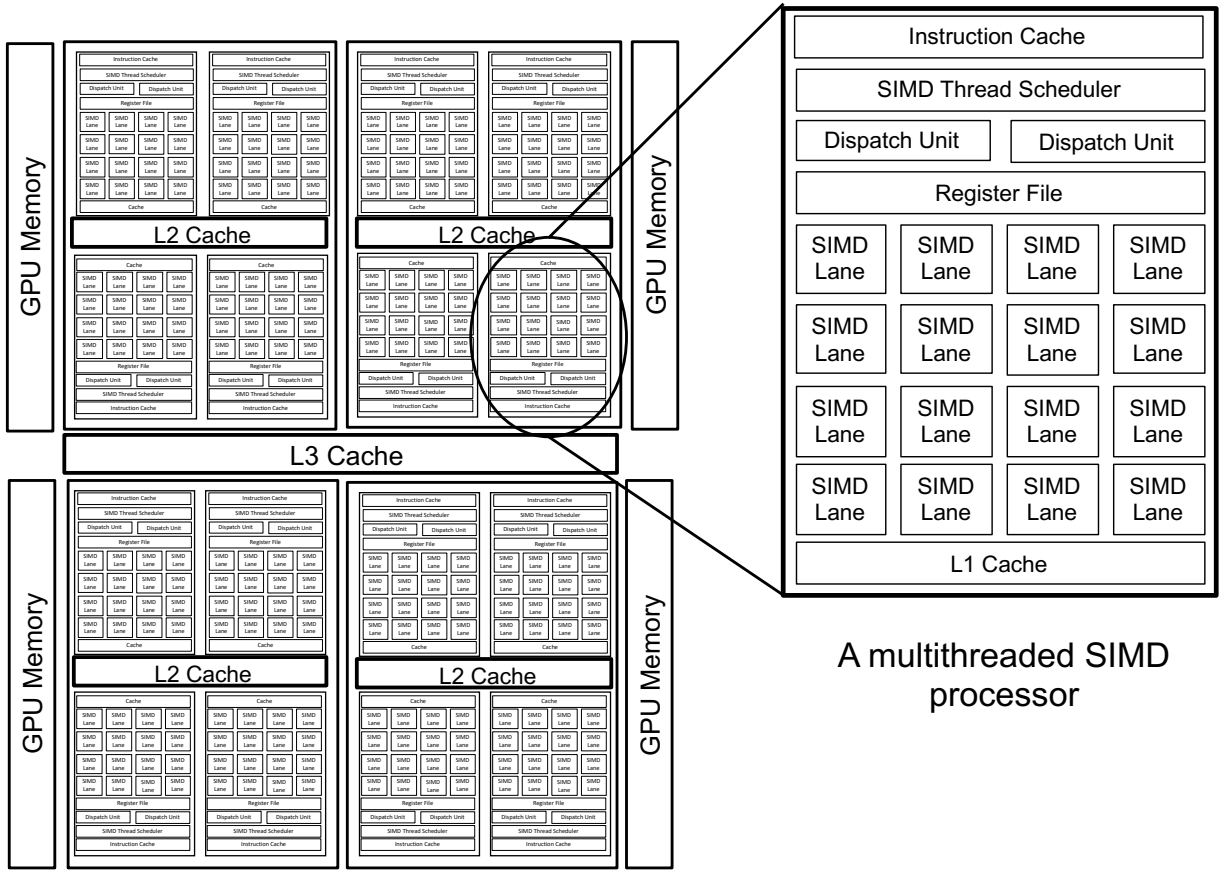
- Use the **target update** construct to transfer data on the fly within a **target data** region or between **target enter/exit data** directives.

Getting the data movement between host memory and device memory is key.

What are the other major issues to consider when optimizing performance?

Occupancy: Keep all the GPU resources busy

- In our “GPU cartoon” we have 16 multithreaded SIMD processors each with 16 SIMD lanes …. For a total of 16^2=256 processing elements.
- You want all resources busy at all times. You do that by keeping excess work for the multithreaded SIMD processors … if they are other busy on some high latency operation, you want a new work-group is ready to be scheduled for execution.
- *Occupancy* having enough work-groups to keep the GPU busy. To support high occupancy, you need many more work-items than SIMD-lanes.



A multithreaded SIMD processor

```
#pragma omp parallel for
for(int i=0;i<N;i++)
  for(int j=0;j<N;j++)
    for(int k=0;i<N;k++)
      *(C+(i*N+j)) += *(A+(i* N +k)) *  *(B+(k* N +j));
```

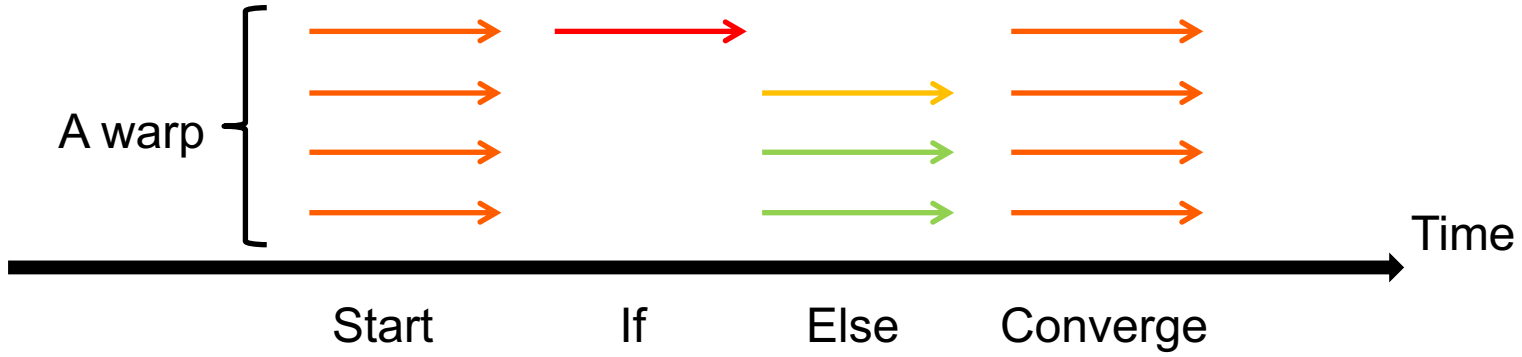
Parallelize i-loop parallelism O(N)

```
#pragma omp parallel for collapse(2)
for(int i=0;i<N;i++)
  for(int j=0;j<N;j++)
    for(int k=0;i<N;k++)
      *(C+(i*N+j)) += *(A+(i* N +k)) *  *(B+(k* N +j));
```

Parallelize combined i/j-loops parallelism O(N^2)

Converged Execution: Single Instruction Multiple Data

- Individual work-items of a warp start together at the same program address
- Each work-item has its own instruction address counter and register state
  - Each work-item is free to branch and execute independently
  - Supports the Single Program Multiple Data (SPMD) pattern.
- Branch behavior
  - Each branch will be executed serially
  - Work-items not following the current branch will be disabled



Converged Execution: Branching

- GPUs tend not to support speculative execution, which means that branch instructions have high latency
- This latency can be hidden by switching to alternative work-items/work-groups, but avoiding branches where possible is still a good idea to improve performance
- When different work-items executing within the same SIMD ALU array take different paths through conditional control flow, we have ***divergent branches*** *(vs.* ***uniform branches****)*
- Divergent branches are bad news: some work-items will stall while waiting for the others to complete
- We can use predication, selection and masking to convert conditional control flow into straight line code and significantly improve the performance of code that has lots of conditional branches

Branching

Conditional execution

```
// Only evaluate expression
// if condition is met
if (a > b)
{
  acc += (a - b*c);
}
```

Selection and masking

```
// Always evaluate expression
// and mask result
temp = (a - b*c);
mask = (a > b ? 1.f : 0.f);
acc += (mask * temp);
```

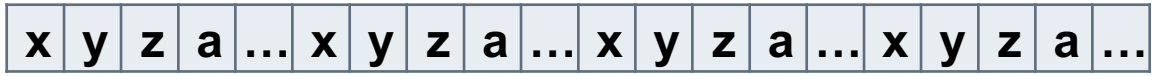
Coalesced memory accesses

- ***Coalesced memory accesses*** are key for high performance code, especially on GPUs
- In principle, it's very simple, but frequently requires transposing or transforming data on the host before sending it to the GPU
- Sometimes this is an issue of Array of Structures vs. Structure of Arrays (AoS vs. SoA)

Memory layout is critical to performance

- Structure of Arrays vs. Array of Structures
  - Array of Structures (AoS) more natural to code:

```
struct Point{ float x, y, z, a; };
Point *Points;
```



  - Structure of Arrays (SoA) suits memory coalescence in vector units

```
struct { float *x, *y, *z, *a; } Points;
```

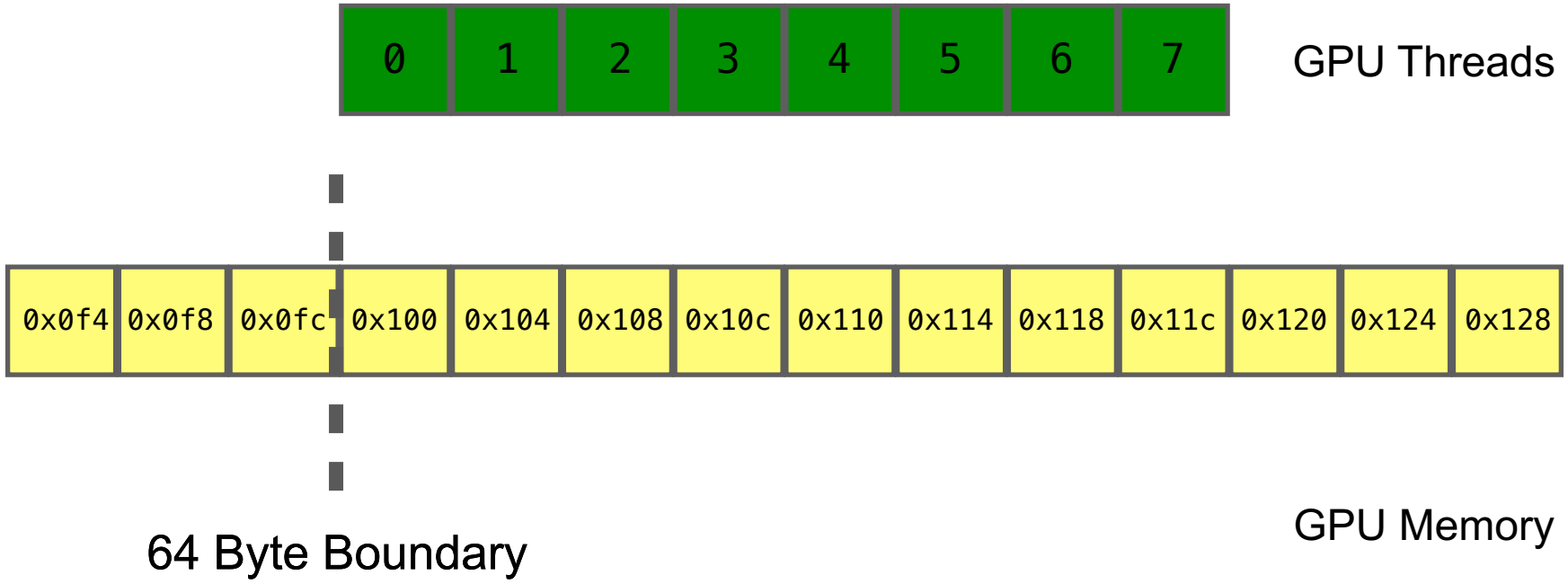
Adjacent work-items/vector-lanes like to access adjacent memory locations

Coalescence

- **Coalesce** - to combine into one
- Coalesced memory accesses are key for high bandwidth
- Simply, it means, if thread *i* accesses memory location *n* then thread *i+1* accesses memory location *n+1*
- In practice, it's not quite as strict…

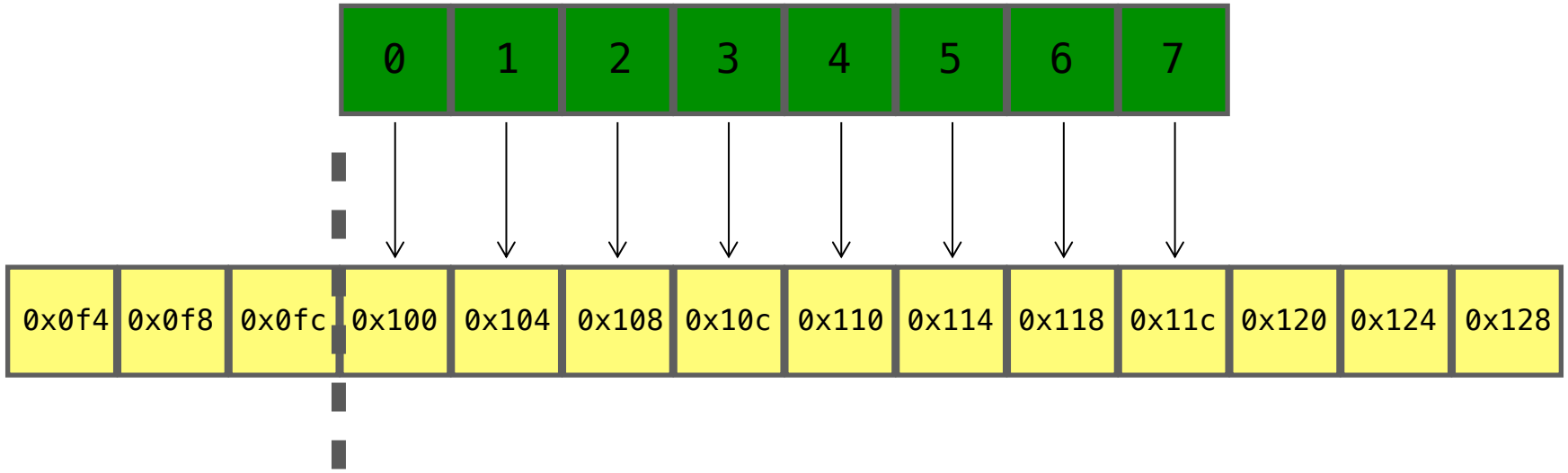
```
for (int id = 0; id < size; id++)
{
  // ideal
     float val1 = memA[id];

  // still pretty good
     const int c = 3;
     float val2 = memA[id + c];

  // stride size is not so good
     float val3 = memA[c*id];

  // terrible
     const int loc =
       some_strange_func(id);

     float val4 = memA[loc];
}
```

Memory access patterns



Memory access patterns

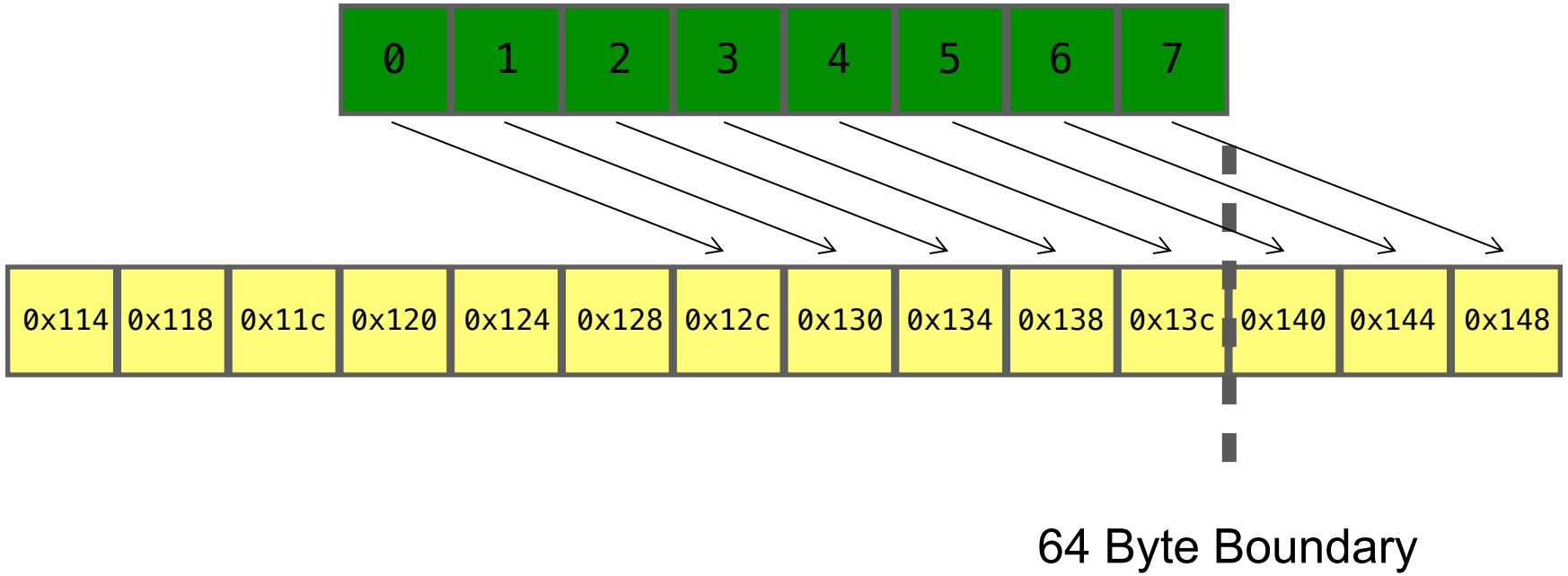
```
float val1 = memA[id];
```



64 Byte Boundary

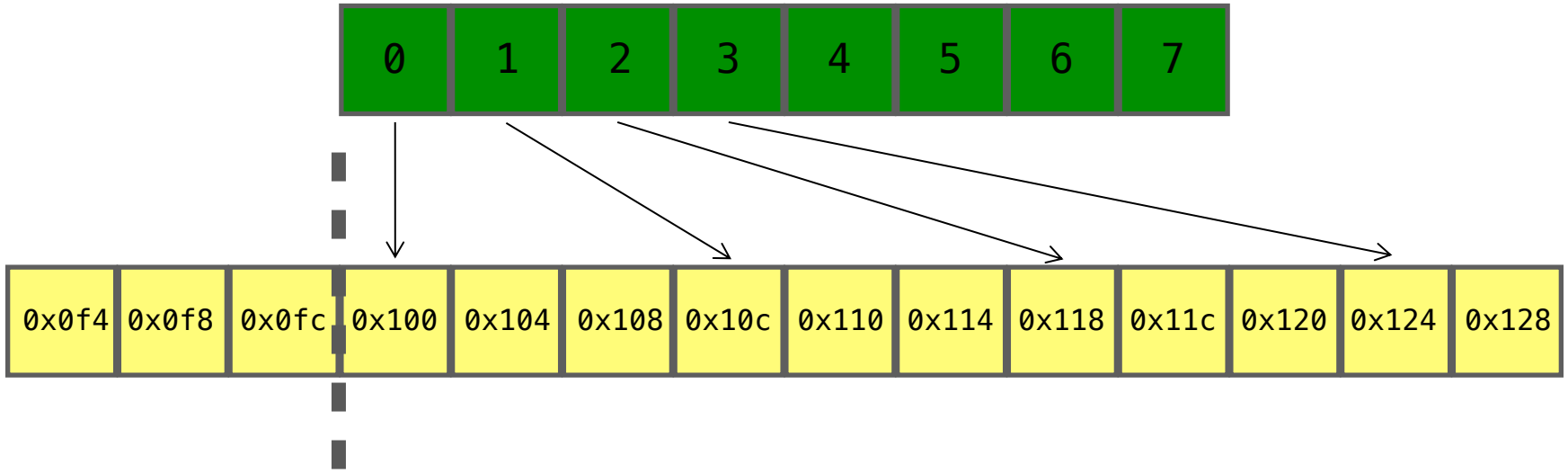
Memory access patterns

```
const int c = 3;
float val2 = memA[id + c];
```



Memory access patterns

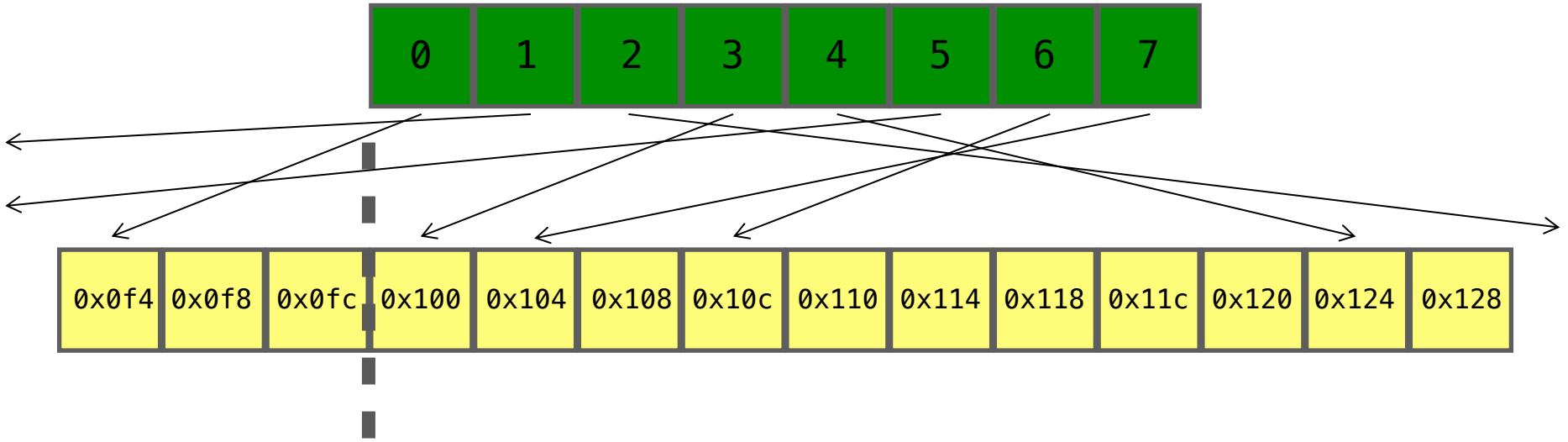
```
float val3 = memA[3*id];
```



Strided access results in multiple memory transactions (and kills throughput)

Memory access patterns

```
const int loc =
  some_strange_func(id);

float val4 = memA[loc];
```



64 Byte Boundary

Exercise

- Optimize the stencil ‘solve’ kernel.
- Start with your code with optimized memory movement from the last exercise.
- Experiment with the optimizations we’ve discussed.
- Focus on the memory access pattern.
- Try different input sizes to see the effect of the optimizations.
- Keep an eye on the solve time as reported by the application.

Solution: collapse + swap loop order

```
// Compute the next timestep, given the current timestep
void solve(const int n, const double alpha, const double dx, const double dt, const double * restrict u,
double * restrict u_tmp) {
  // Finite difference constant multiplier
  const double r = alpha * dt / (dx * dx);
  const double r2 = 1.0 - 4.0*r;

  // Loop over the nxn grid
  #pragma omp target
  #pragma omp loop collapse(2)
  for (int j = 0; j < n; ++j) {
    for (int i = 0; i < n; ++i) {


      // Update the 5-point stencil, using boundary conditions on the edges of the domain.
      // Boundaries are zero because the MMS solution is zero there.
      u_tmp[i+j*n] =  r2 * u[i+j*n] +
      r * ((i < n-1) ? u[i+1+j*n] : 0.0) +
      r * ((i > 0)   ? u[i-1+j*n] : 0.0) +
      r * ((j < n-1) ? u[i+(j+1)*n] : 0.0) +
      r * ((j > 0)   ? u[i+(j-1)*n] : 0.0);
}}}
```

Create more work … to better fill the processing elements of the GPU

Swap the i and j loops so that the i+j*n memory accesses are contiguous

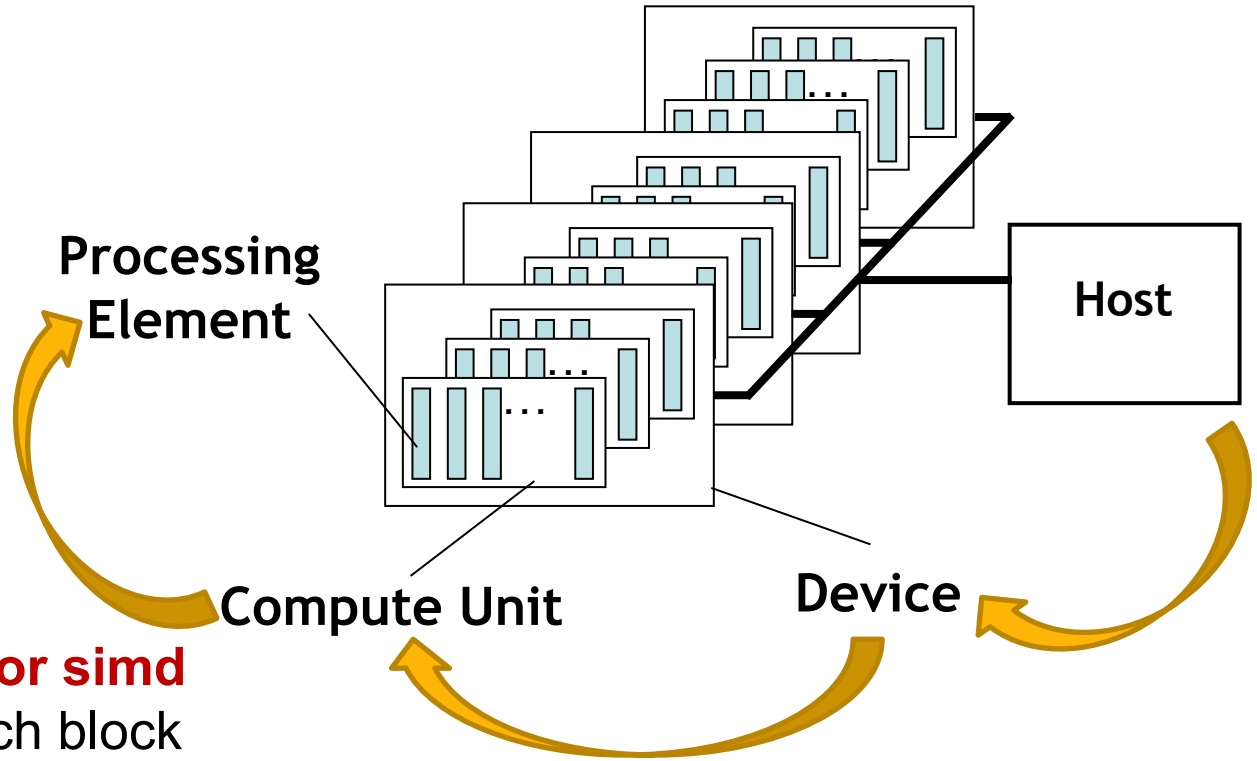
A note about the nowait clause

- Specify dependencies to ensure the **target enter data** finishes *before* the **target** region *sibling* task starts:

```
void init_array(int *A, int N) {
  for (int i = 0; i < N; ++i) A[i] = i;
 #pragma omp target enter data map(to: A[0:N]) nowait depend(out: A)
}

int main(void) {
  int N = 1024; int *A = malloc(sizeof(int) * N);
  init_array(A, N);

  #pragma omp target teams distribute parallel for simd nowait depend(inout: A)
  for (int i = 0; i < N; ++i) A[i] = A[i] * A[i];

  #pragma omp taskwait

  #pragma omp target exit data map(from: A[0:N])
}
```

The loop construct is great, but sometimes you want more control.

Our host/device Platform Model and OpenMP



Parallel for simd to run each block of loop iterations on the processing elements

Teams construct to create a league of teams with one team of threads on each compute unit.

Target construct to get onto a device

Distribute construct to assign blocks of loop iterations to teams.

teams and distribute constructs

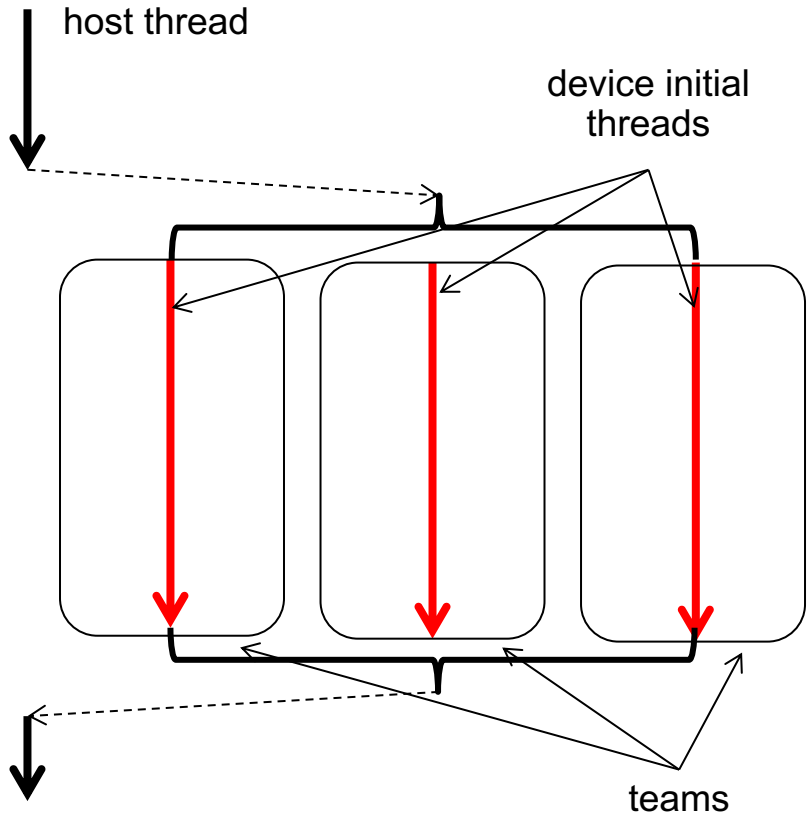
- The **teams** construct
  - Similar to the **parallel** construct
  - It starts a league of thread teams
  - Each team in the league starts as one initial thread – a team of one
  - Threads in different teams cannot synchronize with each other
  - The construct must be “perfectly” nested in a **target** construct

- The **distribute** construct
  - Similar to the **for** construct
  - Loop iterations are workshared across the initial threads in a league
  - No implicit barrier at the end of the construct
  - **dist_schedule(*kind[, chunk_size]*)**
    - If specified, scheduling kind must be static
    - Chunks are distributed in round-robin fashion in chunks of size ***chunk_size***
    - If no chunk size specified, chunks are of (almost) equal size; each team receives at least one chunk

Create a league of teams and distribute a loop among them

- teams construct
- distribute construct

```
#pragma omp target
#pragma omp teams
#pragma omp distribute
 for (i=0;i<N;i++)
   …
```

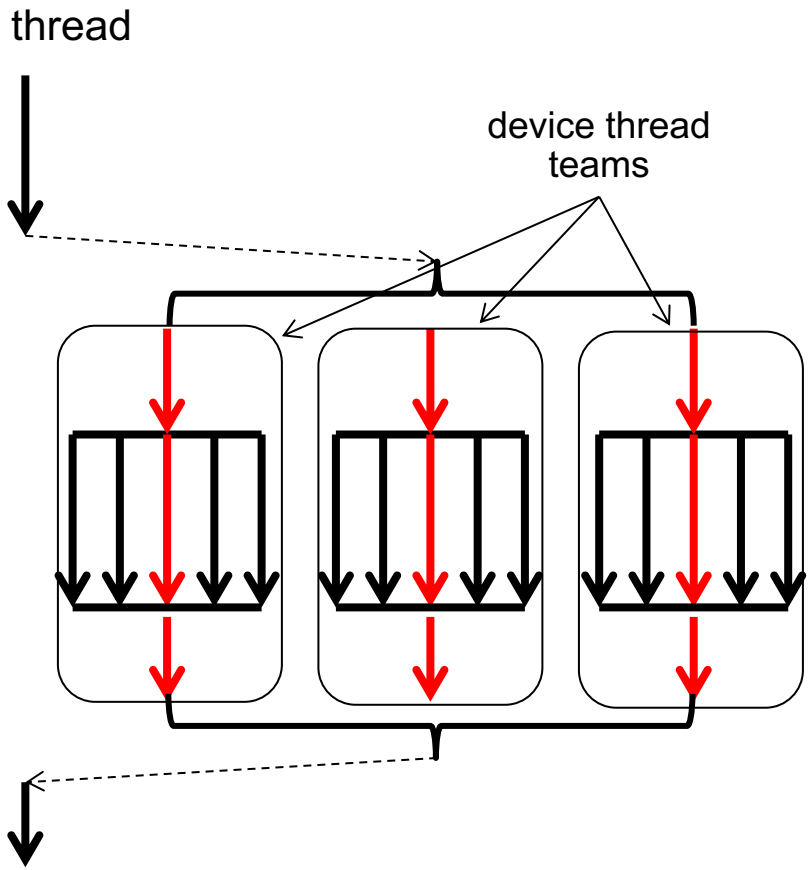


- Transfer execution control to MULTIPLE device initial threads
- Workshare loop iterations across the initial threads.

Create a league of teams and distribute a loop among them and run each team in parallel with its partition of the loop

- teams distribute
- parallel for simd

```
#pragma omp target
#pragma omp teams
#pragma omp distribute
#pragma omp parallel for simd
 for (i=0;i<N;i++)
    …
```

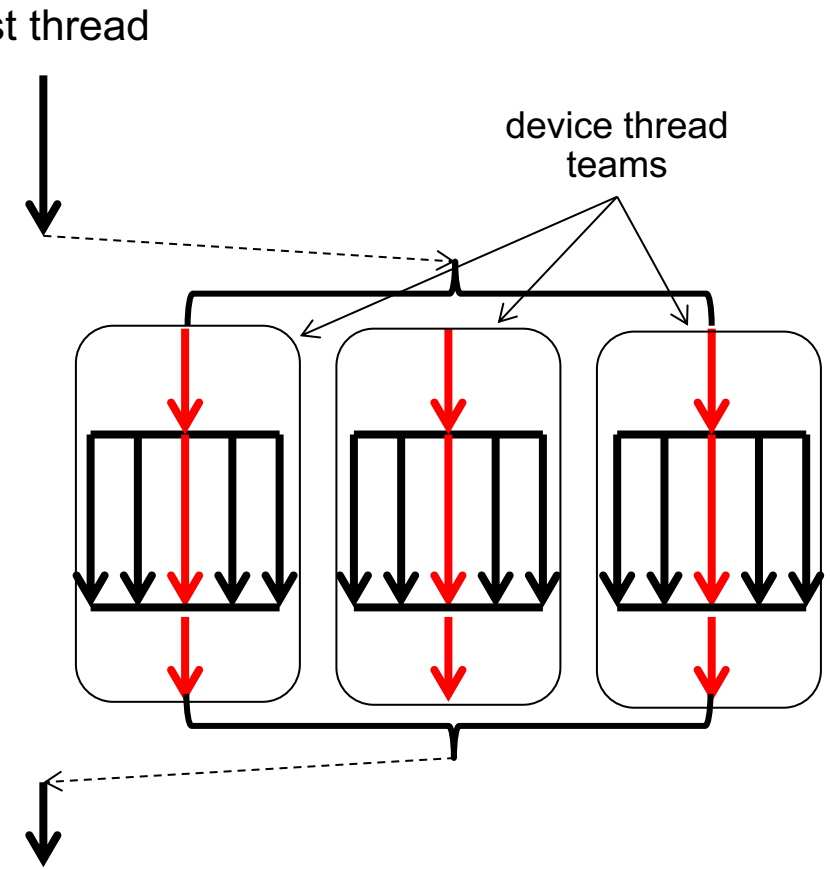


- Transfer execution control to MULTIPLE device initial threads
  - Workshare loop iterations across the initial threads (teams distribute)
- Each initial thread becomes the primary* thread in a thread team
  - Workshare loop iterations across the threads in a team (parallel for)

Create a league of teams and distribute a loop among them and run each team in parallel with its partition of the loop

- loop

```
#pragma omp target
#pragma omp teams
#pragma omp loop
 for (i=0;i<N;i++)
    …
```



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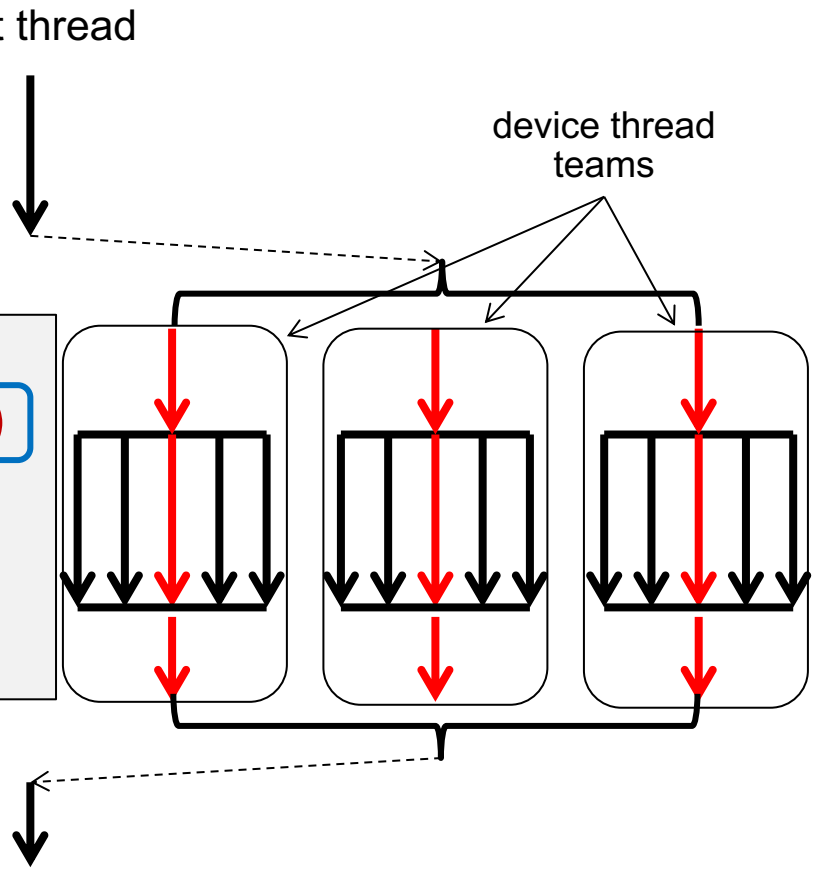
Create a league of teams and distribute a loop among them and run each team in parallel with its partition of the loop

- teams distribute
- parallel for simd

```
#pragma omp target
#pragma omp teams num_teams(3) thread_limit(5)
#pragma omp distribute
#pragma omp parallel for simd
 for (i=0;i<N;i++)
   …
```

Explicit control of number and size of teams



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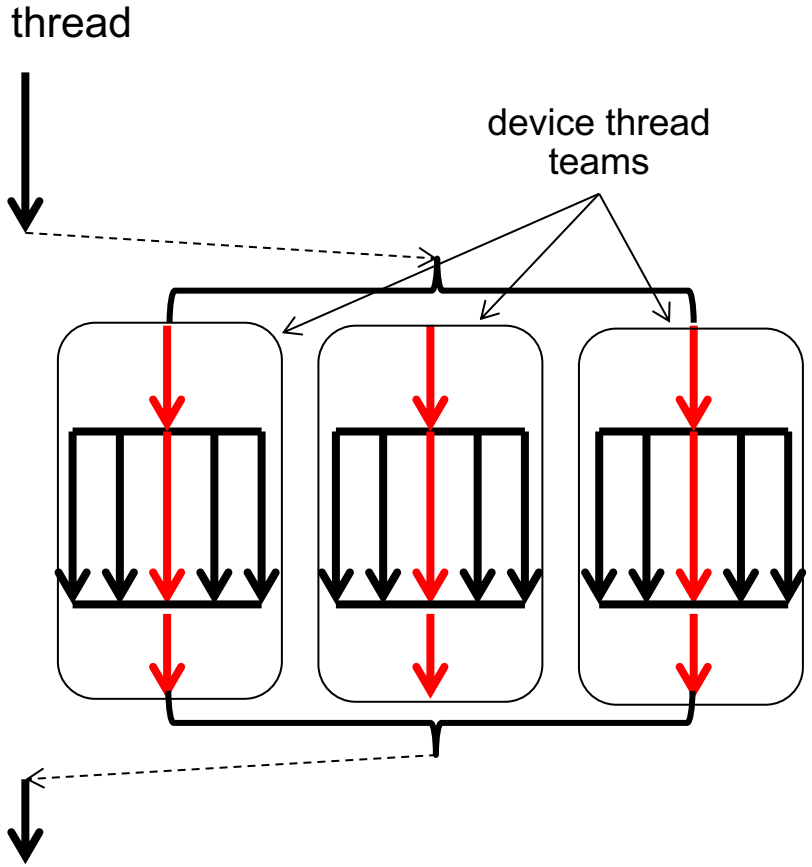
Create a league of teams and distribute a loop among them and run each team in parallel with its partition of the loop

- Combined construct

```
#pragma omp target  teams loop
for (i=0;i<N;i++)
    …
```



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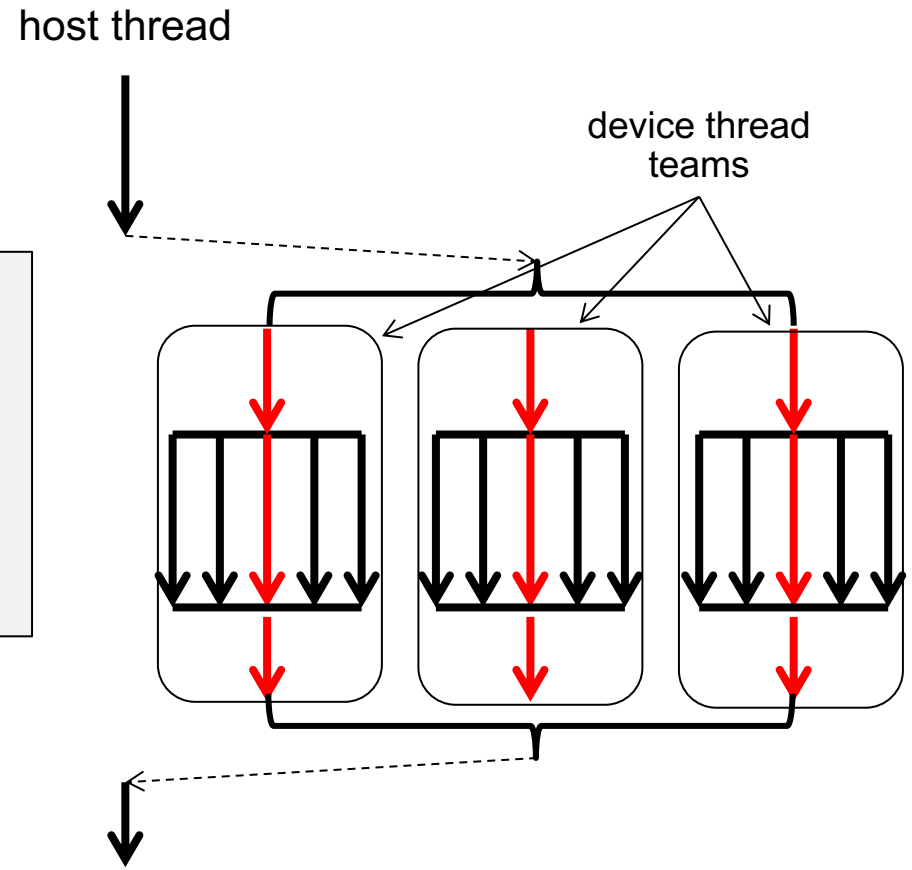
Create a league of teams and distribute a loop among them and run each team in parallel with its partition of the loop

- teams distribute
- parallel for simd

Works with nested loops as well

```
#pragma omp target
#pragma omp teams distribute
 for (i=0;i<N;i++)
 #pragma omp parallel for simd
 for (j=0;j<M;i++)
   ...
```



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- Each initial thread becomes the primary* thread in a thread team
  - Workshare loop iterations across the threads in a team (parallel for)

There is MUCH more … beyond what have time to cover

- Do as much as you can with a simple loop construct. It's portable and as compilers improve over time, it will keep up with compiler driven performance improvements.
- But sometimes you need more:
  - Control over number of teams in a league and the size of the teams
  - Explicit scheduling of loop iterations onto the the teams
  - Management of data movement across the memory hierarchy: global vs. shared vs. private …
  - Calling optimized math libraries (such as cuBLAS)
  - Multi-device programming
  - Asynchrony
- Ultimately, you may need to master all those advanced features of GPU programming. But start with loop. Start with how data on the host maps onto the device (i.e. the GPU). Master that level of GPU programming before worrying about the complex stuff.

This is the end … well almost the end.

Let’s wrap up with a few high-level comments about the state of GPU programming more generally

SIMT Programming models: it's more than just OpenMP

- CUDA:
  - Released ~2006. Made GPGPU programming "mainstream" and continues to drive innovation in SIMT programming.
    - Downside: proprietary to NVIDIA
- OpenCL:
  - Open Standard for SIMIT programming created by Apple, Intel, NVIDIA, AMD, and others. 1st release in 2009.
  - Supports CPUs, GPUs, FPGAs, and DSP chips. The leading cross platform SIMT model.
    - Downside: extreme portability means verbose API. Painfully low level especially for the host-program.
- Sycl:
  - C++ abstraction layer implements SIMT model with kernels as lambdas. Closely aligned with OpenCL. 1st release 2014
    - Downside: Cross platform implementations only emerging recently.
- Directive driven programming models:
  - **OpenACC**: they split from an OpenMP working group to create a competing directive driven API emphasizing descriptive (rather than prescriptive) semantics.
    - ~~Downside: NOT an Open Standard. Controlled by NVIDIA.~~ → They've made it more open, but it still doesn't add anything you can't do in OpenMP
  - **OpenMP**: Mixes multithreading and SIMT. Semantics are prescriptive which makes it more verbose. A truly Open standard supported by all the key GPU players. And with the loop construct … its now prescriptive (hence there is no longer any reason for OpenACC to exist)

Vector addition with CUDA

```
// Compute sum of length-N vectors: C = A + B
void __global__
vecAdd (float* a, float* b, float* c, int N) {
    int i = blockIdx.x * blockDim.x + threadIdx.x;
    if (i < N) c[i] = a[i] + b[i];
}

int main () {
    int N = ... ;
    float *a, *b, *c;
    cudaMalloc (&a,  sizeof(float) * N);
// ... allocate other arrays (b and c), fill with data

  // Use thread blocks with 256 threads each
    vecAdd <<< (N+255)/256, 256 >>> (a, b, c, N);
}
```

CUDA kernel as function

Unified shared memory … allocate on host, visible on device too

Enqueue the kernel to execute on the Grid

Vector addition with SYCL

```
// Compute sum of length-N vectors: C = A + B
#include <CL/sycl.hpp>

int main () {
    int N = ... ;
    float *a, *b, *c;
    sycl::queue q;
    *a = (float *)sycl::malloc_shared(N * sizeof(float), q);
  // ... allocate other arrays (b and c), fill with data

        q.parallel_for(sycl::range<1>{N},
                [=](sycl::id<1> i) {
                  c[i] = a[i] + b[i];
                });
         q.wait();
}
```

Create a queue for SYCL commands

Unified shared memory … allocate on host, visible on device too

Kernel as a C++ Lambda function

[=] means capture external variables by value.

Vector addition with OpenACC

- Let's add two vectors together …. C = A + B

```
void vadd(int n,
          const float *a,
          const float *b,
          float *restrict c)
{
  int i;
 #pragma acc parallel loop
  for (i=0; i<n; i++)
    c[i] = a[i] + b[i];
}
int main(){
float *a, *b, *c;  int n = 10000;
// allocate and fill a and b

    vadd(n, a, b, c);

}
```

Assure the compiler that c is not aliased with other pointers

Turn the loop into a kernel, move data to a device, and launch the kernel.

Host waits here until the kernel is done. Then the output array c is copied back to the host.

Why so many ways to do the same thing?

- The parallel programming model people have failed you …
  - It's more fun to create something new in your own closed-community that work across vendors to create a portable API
- The hardware vendors have failed you …
  - Don't you love my "walled garden"? It's so nice here, programmers, just don't even think of going to some other platform since your code is not portable.
- The standards community has failed you …
  - Standards are great, but they move too slow. OpenACC stabbed OpenMP in the back and I'm pissed, but their comments at the time were spot-on (OpenMP was moving so slow … they just couldn't wait).
- The applications community failed themselves …
  - If you don't commit to a standard and use "the next cool thing" you end up with the diversity of overlapping options we have today. Think about what happened with OpenMP and MPI.

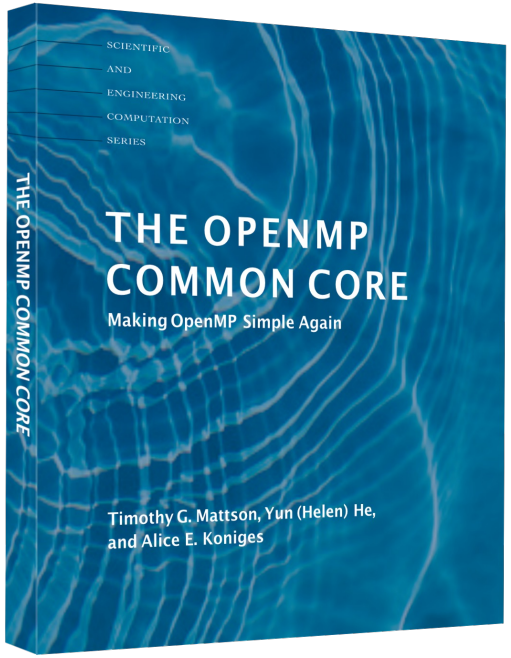
Summary

- Parallel computing is fun … but it can be hard.
- Fortunately, if you stick to the Big-3 and the core patterns of parallel computing for HPC, it's not too overwhelming
  - The big 3: MPI, OpenMP, and "a GPU programming model"
  - Key Patterns: SPMD, loop level parallelism, geometric decomposition, divide and conquer, and SIMT
- Some day we'll automate the hard-parts with Machine Programming, but that may be 10 years!!!!

To learn more about OpenMP

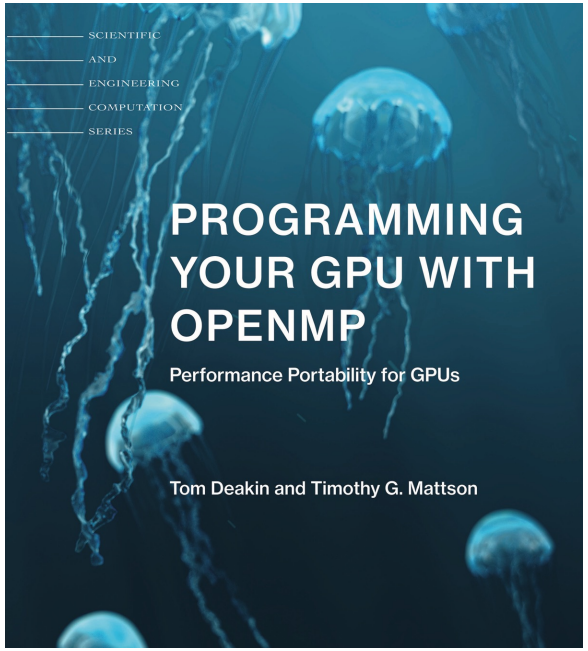
The OpenMP web site has a great deal of material to help you with OpenMP www.openmp.org
Reading the spec is painful … but each spec has a collection of examples. Study the examples, don't try to read the specs

Since the specs are written ONLY for implementors … programmers need the OpenMP Books to master OpenMP.



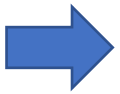
Start here … learn the basics and build a foundation for the future

Learn advanced features in OpenMP including tasking and GPU programming (up to version 4.5)



Learn all the details of GPU programming with OpenMP
(up to version 5.2)

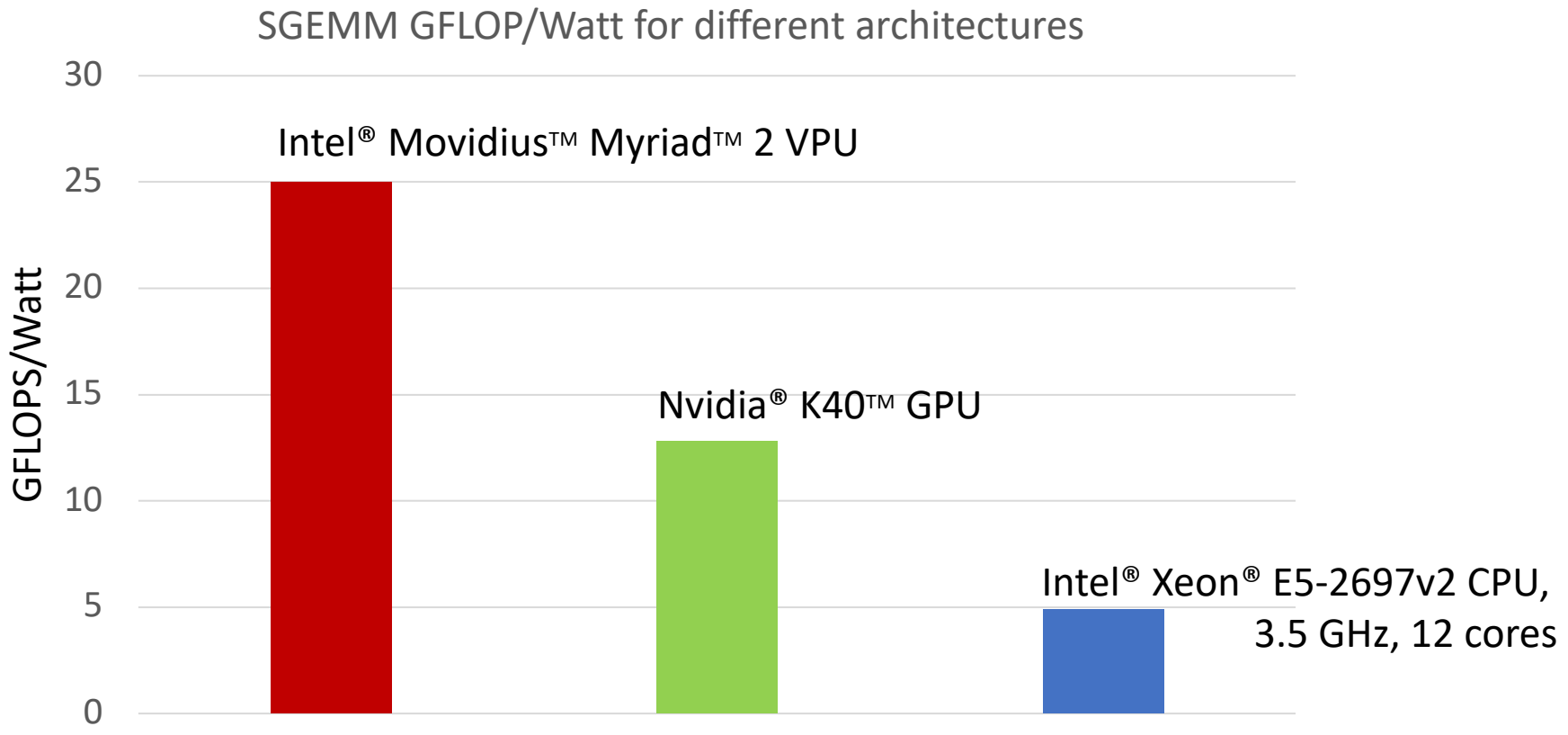
Backup … and a bit of extra content



- The future of parallel programming
- The Jacobi solver case study
- Writing functions to call from inside a kernel

If you care about power, the world is heterogeneous?

Specialized processors doing operations suited to their architecture are more efficient than general purpose processors.

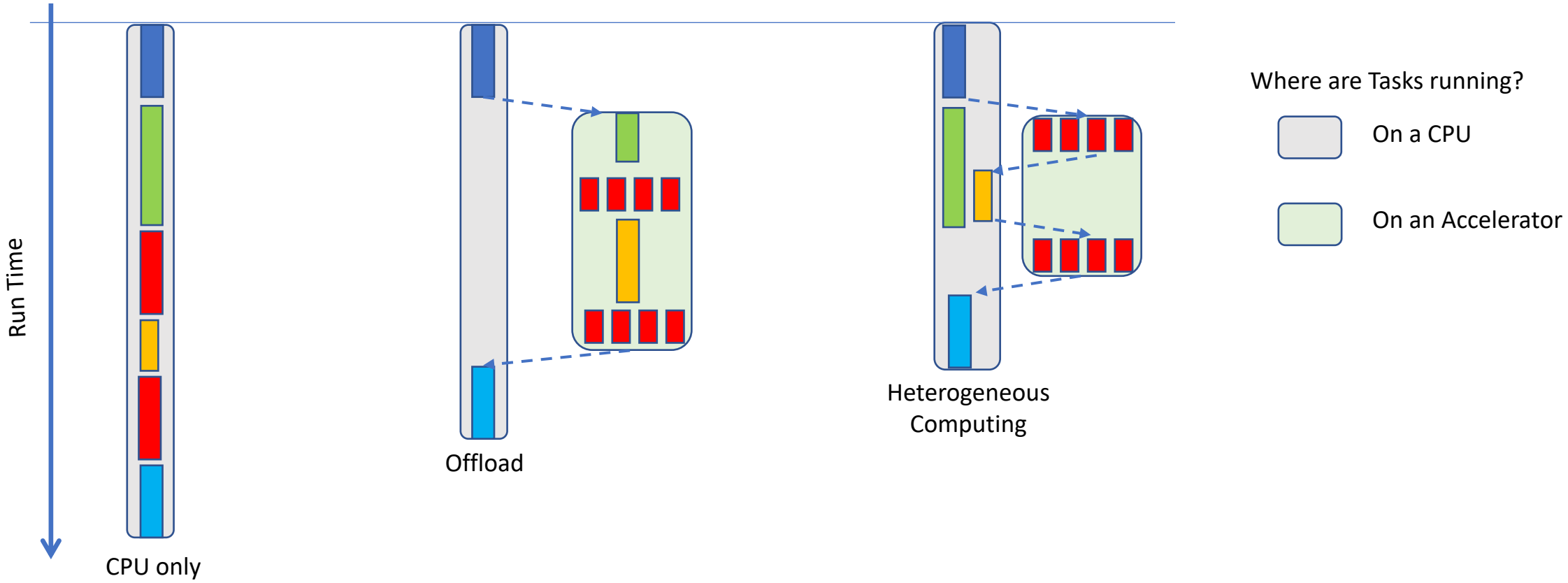


Hence, future systems will be increasingly heterogeneous … GPUs, CPUs, FPGAs, and a wide range of accelerators

Source: Suyash Bakshi and Lennart Johnsson, "A Highly Efficient SGEMM Implementation using DMA on the Intel/Movidius Myriad-2. IEEE International Symposium on Computer Architecture and High Performance Computing, 2020

Offload vs. Heterogeneous computing

- **Offload**: The CPU moves work to an accelerator and waits for the answer.
- **Heterogeneous Computing**: Run sub-problems in parallel on the hardware best suited to them.



Example: Single-cell RNA-Seq benchmark (SCANPY)

- SCANPY … a widely used tool for studying gene expression. All data are elapsed time in seconds
- We started with results from an Nvidia blog (Example 2 from link), optimized code for one socket of Intel® Xeon® 8380 CPU and then "simulated" heterogeneous computing result by taking the faster of CPU and GPU execution times.

Pipeline stages	64 vCPUs n1-highmem-64 (off-the-shelf Python)	A100 40Gb (Clara Parabricks)	ICX-1s, 40 cores (**optimized by Intel**)	*"Simulated"* heterogeneous A100 & ICS-1s 40 cores
Data Loading & Preprocessing	1120	475	15.7	15.7
PCA	44	17.8	5.0	5.0
T-SNE	6509	37	205.6	37
K-means (single iteration)	148	2	7.1	2
KNN	154	62	59.8	59.8
UMAP	2571	21	84.5	21
Louvain clustering	1153	2.4	6.0	2.4
Leiden clustering	6345	1.7	28.4	1.7
Reanalysis of subgroup	255	17.9	22.5	17.9
Rest	39	49.2	49.0	49.0
End-to-End runtime	**18338**	**686**	**483.6**	**211.5**

Redacted

Imagine mixing the best of the CPU and GPU numbers. What would the performance look like?

Lessons learned:

- Be careful comparing unoptimized python to hand-tuned CUDA code
- GPUs are great. So are CPUs if you fully utilize all the cores and vector units.
- What you really want is the best of both worlds. **You want heterogeneous computing!**

See Backup for workloads and configurations. Results may vary.

Clara Parabricks: Nvidia solution stack built on RAPIDS for healthcare applications

https://github.com/clara-parabricks/rapids-single-cell-examples

github repository as of Dec 16, 2020

This column shows the potential of heterogenous computing. We ignored extra communication and synchronization overhead, so actual runtimes would be slightly greater.

Source: Github repository as of Dec 16, 2020 - Example 2: Single-cell RNA-seq of 1.3 Million Mouse Brain Cells comparing CPU (n1-highmem-64 64 vCPUs) vs GPU (n1-highmem-16. https://github.com/clara-parabricks/rapids-single-cell-examples. Intel does not control or audit third-party data. You should consult other sources to evaluate accuracy.

1S Ice Lake: See Backup for workloads and configurations. Results may vary.

Five Epochs of Distributed Computing*

Epoch starting date	Defining limitations	Application	Interaction time and Network performance	Capability
First 1970	Rare connections to expensive computers	FTP, telnet, email	100 ms Low bandwidth high latency	People to computers
Second 1984	I/O wall, disks can't keep up	RPC, Client Server	10 ms 10 mbps	Computer to computer
Third 1990	Networking wall	MPP HPC, three-tier datacenter networks	1 ms 100 mbs → 1 Gbs	Services to services
Fourth 2000	Dennard scaling wall … per core plateau	Web search, planet-scale services	100 μs 10 Gbps flash	People to people
Fifth 2015	Per socket wall … accelerators take off	Machine Learning, data centric computing	10 μs 200 Gbps → 1 Tbps	People to insights

*The five Epochs of distributed computing, Amin Vahdat of Google: SIGCOMM Lifetime achievement award keynote, 2020.

The Eight Fallacies of Distributed Computing

(Peter Deutsch of Sun Microsystems, 1994 … item 8 added in 1997 by James Gosling)

Essentially everyone, when they first build a distributed application, makes the following eight assumptions. All prove to be false in the long run and all cause *big* trouble and *painful* learning experiences.

1. The network is reliable
2. Latency is zero
3. Bandwidth is infinite
4. The network is secure
5. Topology doesn't change
6. There is one administrator
7. Transport cost is zero
8. The network is homogeneous

https://en.wikipedia.org/wiki/Fallacies_of_distributed_computing

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1. The network is reliable
2. Latency is low and fixed
3. Bandwidth is high and fixed
4. The network is secure
5. Topology doesn't change
6. There is one administrator
7. Transport cost is negligible
8. The network is homogeneous

https://en.wikipedia.org/wiki/Fallacies_of_distributed_computing

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Cloud

1. ~~The network is reliable~~
2. ~~Latency is low and fixed~~
3. ~~Bandwidth is high and fixed~~
4. ~~The network is secure~~
5. ~~Topology doesn't change~~
6. ~~There is one administrator~~
7. ~~Transport cost is negligible~~
8. ~~The network is homogeneous~~

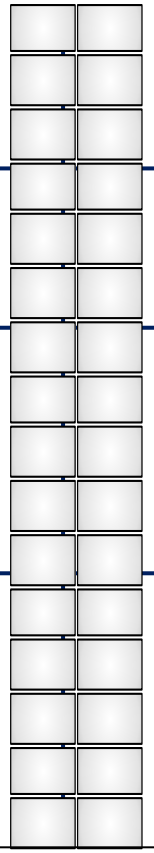
HPC Cluster

1. The network is reliable
2. Latency is low and fixed
3. Bandwidth is high and fixed
4. The network is secure
5. Topology doesn't change
6. There is one administrator
7. ~~Transport cost is negligible~~
8. The network is homogeneous

https://en.wikipedia.org/wiki/Fallacies_of_distributed_computing

The three domains of parallel programming

Platform*	Laptop or server	HPC Cluster	Cloud
Execution Agent	Threads	Processes	Microservices
Memory	Single Address Space	Distributed memory, local memory owned by individual processes	Distributed object store (in memory) backed by a persistent storage system
Typical Execution Pattern	Fork-join	SPMD	Event driven tasks, FaaS, and Actors



Laptop/server and cluster models work well together.

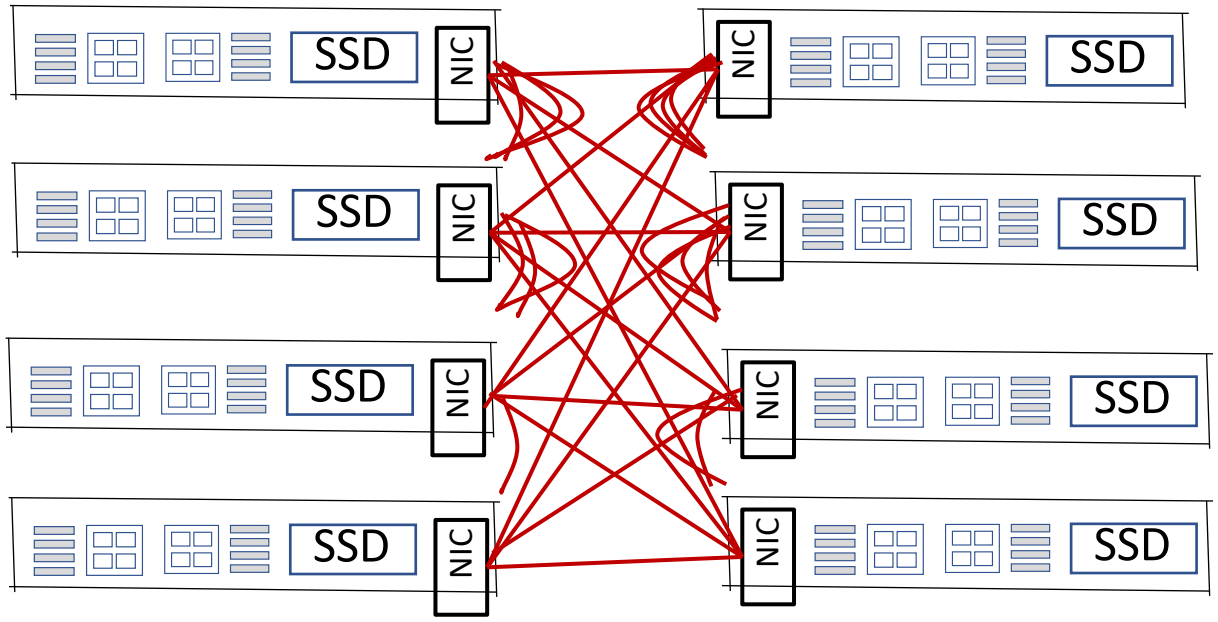
An impenetrable wall separates them from the cloud-native world

The sixth Epoch of Distributed Computing

Epoch starting date	Defining limitations	Application	Interaction time and Network performance	Capability
First 1970	Rare connections to expensive computers	FTP, telnet, email	100 ms Low bandwidth high latency	People to computers
Second 1984	I/O wall, disks can't keep up	RPC, Client Server	10 ms 10 mbps	Computer to computer
Third 1990	Networking wall	MPP HPC, three-tier datacenter networks	1 ms 100 mbs → 1 Gbs	Services to services
Fourth 2000	Dennard Scaling Wall … per core plateau	Web search, planet-scale services	100 μs 10 Gbps flash	People to people
Fifth 2015	Per socket wall … accelerators take off	Machine Learning, data centric computing	10 μs 200 Gbps → 1 Tbps	People to insights
Sixth 2025	Speed of light	Dynamic, real-time AI, integrated from data-center to the edge with SDE*	100 ns 10 Tbs	People to experiences

* SDE: Software defined Everything, i.e. software defined networking, software defined infrastructure, software defined servers ... All at the same time … to dynamically construct systems to meet the needs of workloads.

Networking technology… replace generic data center network with a cluster of cliques



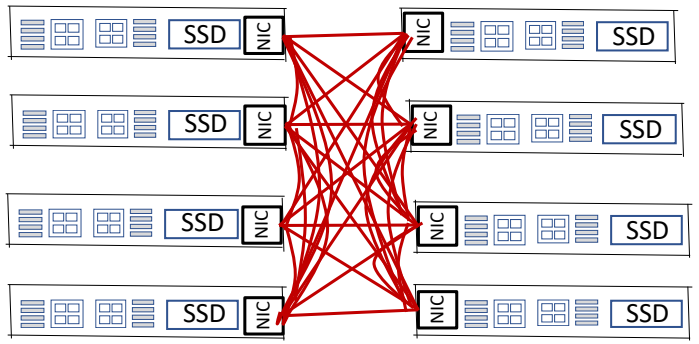
A clique: A graph where every vertex is connected to every other vertex

A Clique: a network of diameter one with
$O(\frac{1}{4}N^2)$ bisection bandwidth

Combine with next generation optical networks to hit latencies of 100 ns

Latencies every engineer should know …

L1 cache reference 1.5 ns
L2 cache reference 5 ns
Branch misprediction 6 ns
Uncontended mutex lock/unlock 20 ns
L3 cache reference 25 ns
Main memory reference 100 ns
“Far memory”/Fast NVM reference 1,000 ns (1us)
Read 1 MB sequentially from memory 12,000 ns (12 us)
SSD Random Read 100,000 ns (100 us)
Read 1 MB bytes sequentially from SSD 500,000 ns (500 us)
Read 1 MB sequentially from 10Gbps network 1,000,000 ns (1 ms)
Read 1 MB sequentially from disk 10,000,000 ns (10 ms)
Disk seek 10,000,000 ns (10 ms)
Send packet California→Netherlands→California (150 ms)



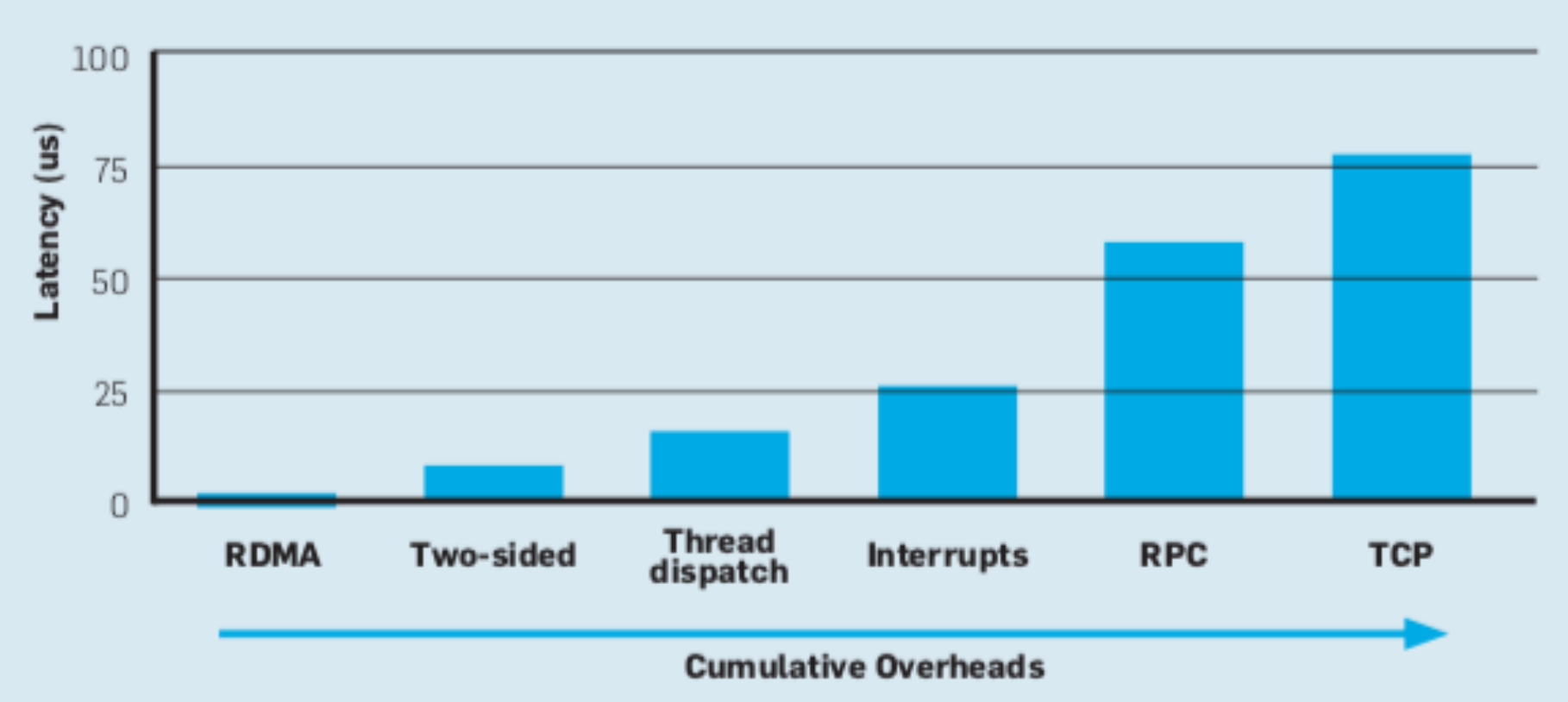
A cluster of nodes with a Clique network topology and low latency optical network…

Yields one hop network latencies on par with DRAM access latencies.

Source: **The Datacenter as a Computer: Designing Warehouse-Scale Machines**, Luiz Andre Barroso, Urs Holzle, Parthasarathy Ranganathan, 3rd edition, Morgan & Claypool, 2019.

Take out the big stuff & you're left with lots of µs overheads

All those SW overheads add up … like bricks that combine to build a networking-wall … turning a 2 µs network into a 100 µs network…

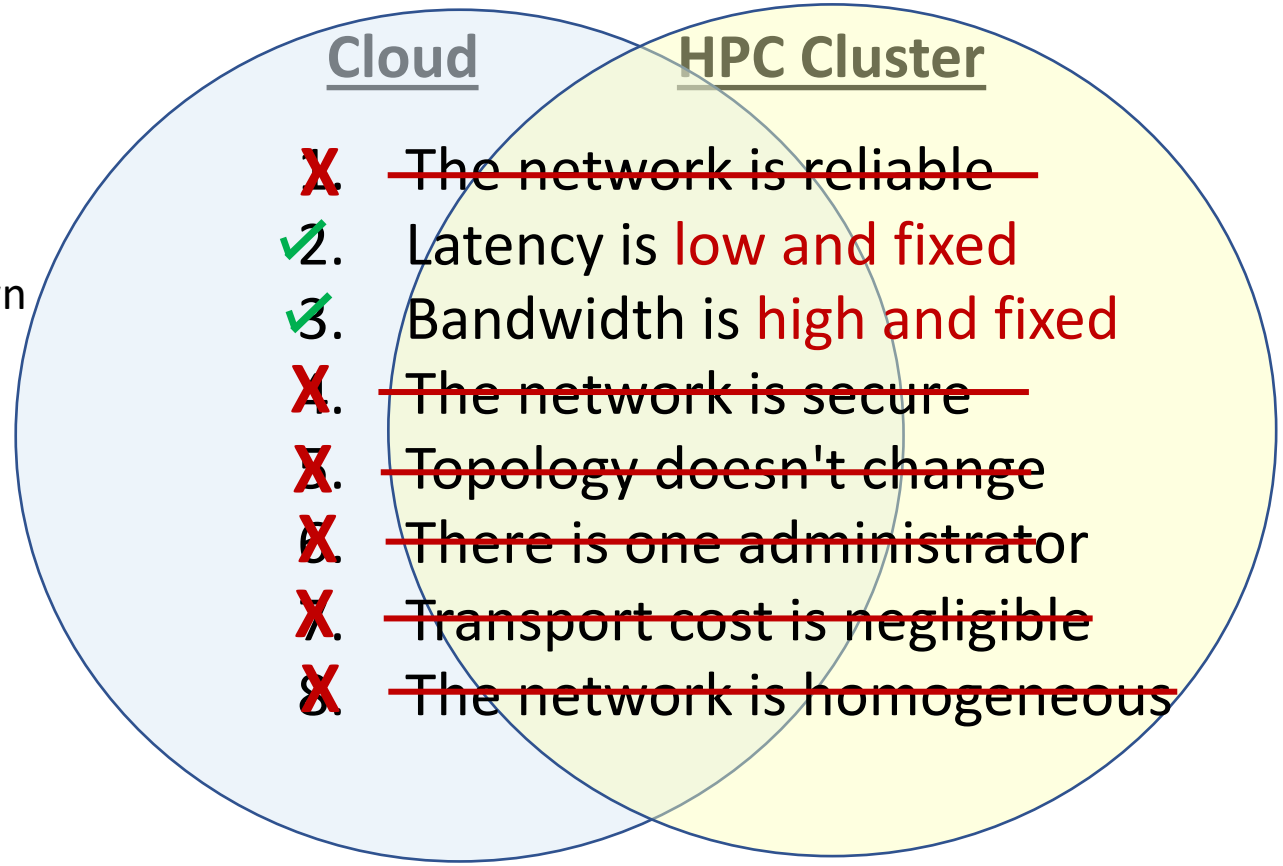


Computer Scientists need to rethink system SW stacks to minimize latencies … fast RDMA, reduce sync contention, low latency interrupt handlers, and more …. All to hit O(µs) latencies.

Source: Fig 1 from "Attack of the Killer Microseconds", Barroso, Marty, Patterson, and Ranganathan, Comm ACM vol 60, # 4, p. 48, 2017

In the sixth Epoch of Distributed Computing, cloud and cluster overlap … or even merge!

Chip-to-chip optical networks push latency down and bandwidth up



Data Streaming Accelerator reduces tail latency.

P4/P5/P6 + Infrastructure Processing Units drive down latency and reduces jitter

With Low Latencies, high bandwidths and stable performance, we can do loosely synchronous and synchronous applications in the cloud. The economics of the cloud vs dedicated HPC clusters means the cloud will dominate HPC

HPC applications will need to change to deal with reliability and network inhomogeneities.

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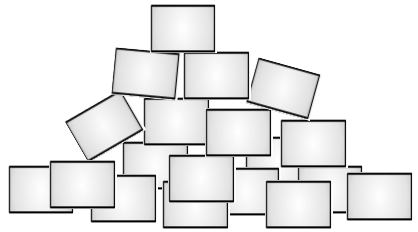
Advances in networking technology plus low-overhead software stacks optimized to reduce tail-latency will shatter this wall



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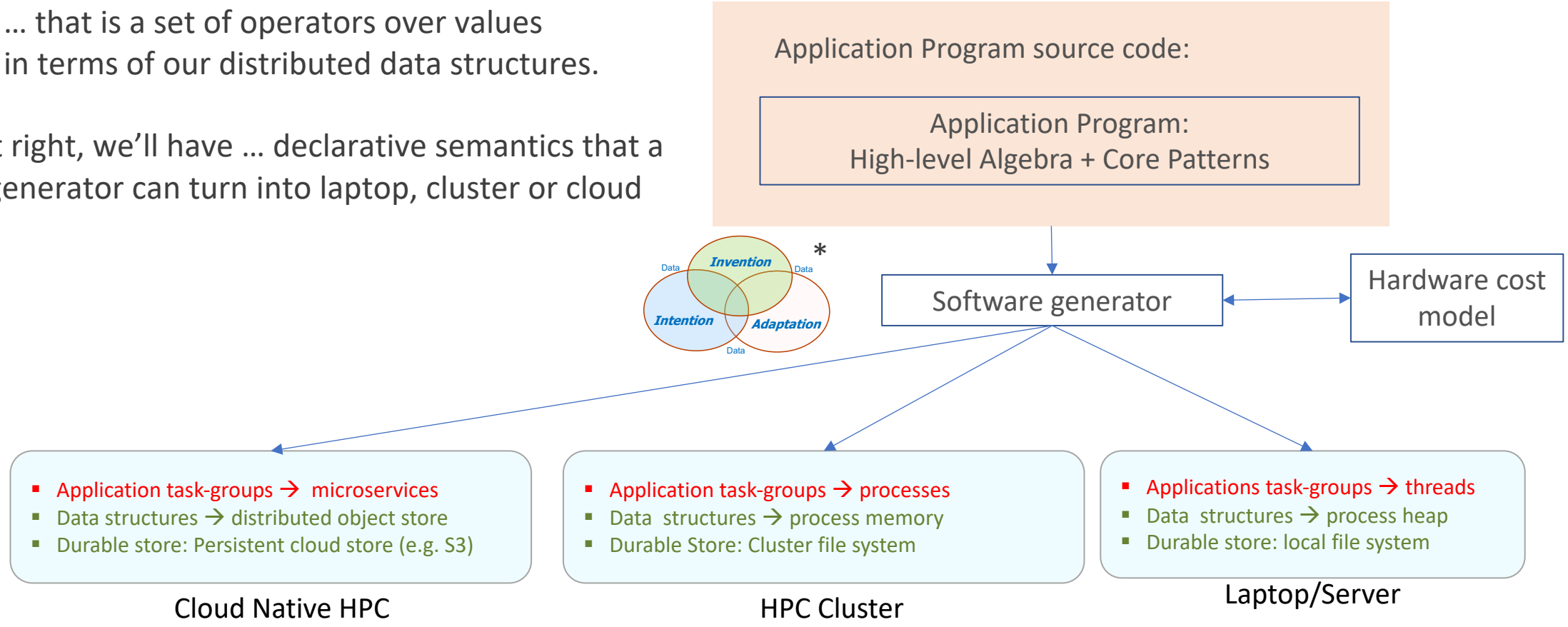
There will always be a need for top-end scalable systems in supercomputer centers, but economics will push the bulk of scientific computing into the cloud.

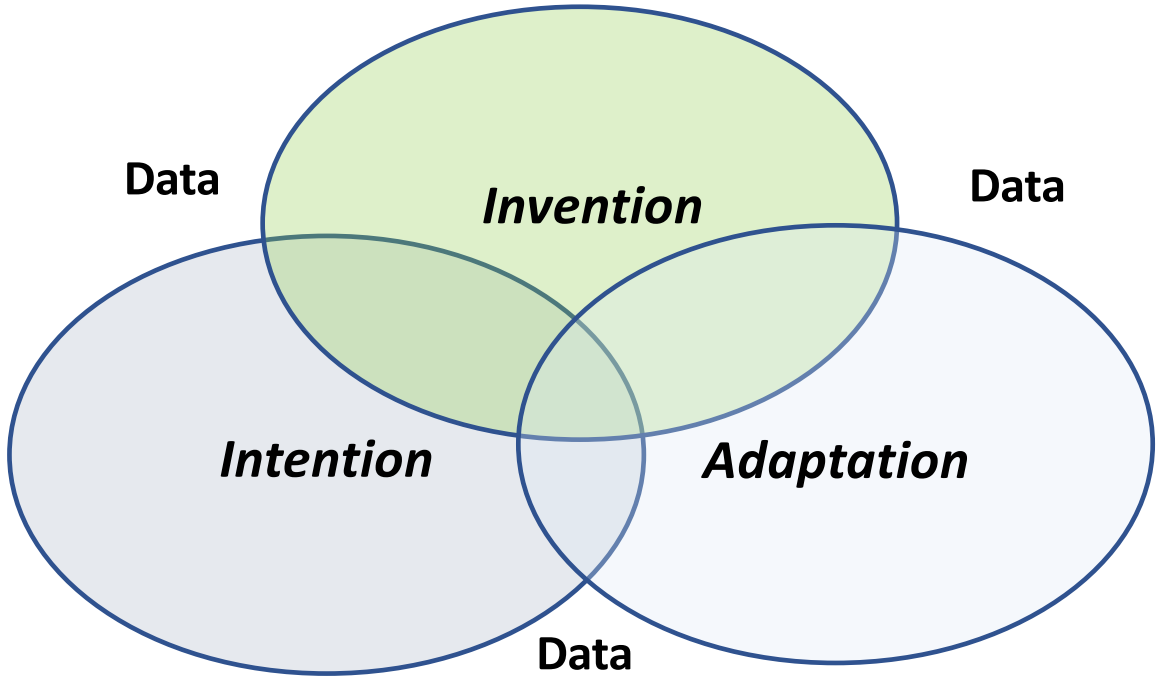
One codebase → many systems

- Performance, Productivity AND Portability … the database people "did it" with relational algebras and SQL.
- We can do it too with algebras over distributed data structures … that is a set of operators over values expressed in terms of our distributed data structures.
- If we get it right, we'll have … declarative semantics that a software generator can turn into laptop, cluster or cloud programs.



*This is the logo of the machine programming research program I help lead inside Intel Labs

The Three Pillars of Machine Programming (MP)



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Armando Solar-Lezama, MIT
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Joshua B Tenenbaum, MIT
Tim Mattson, Intel Labs

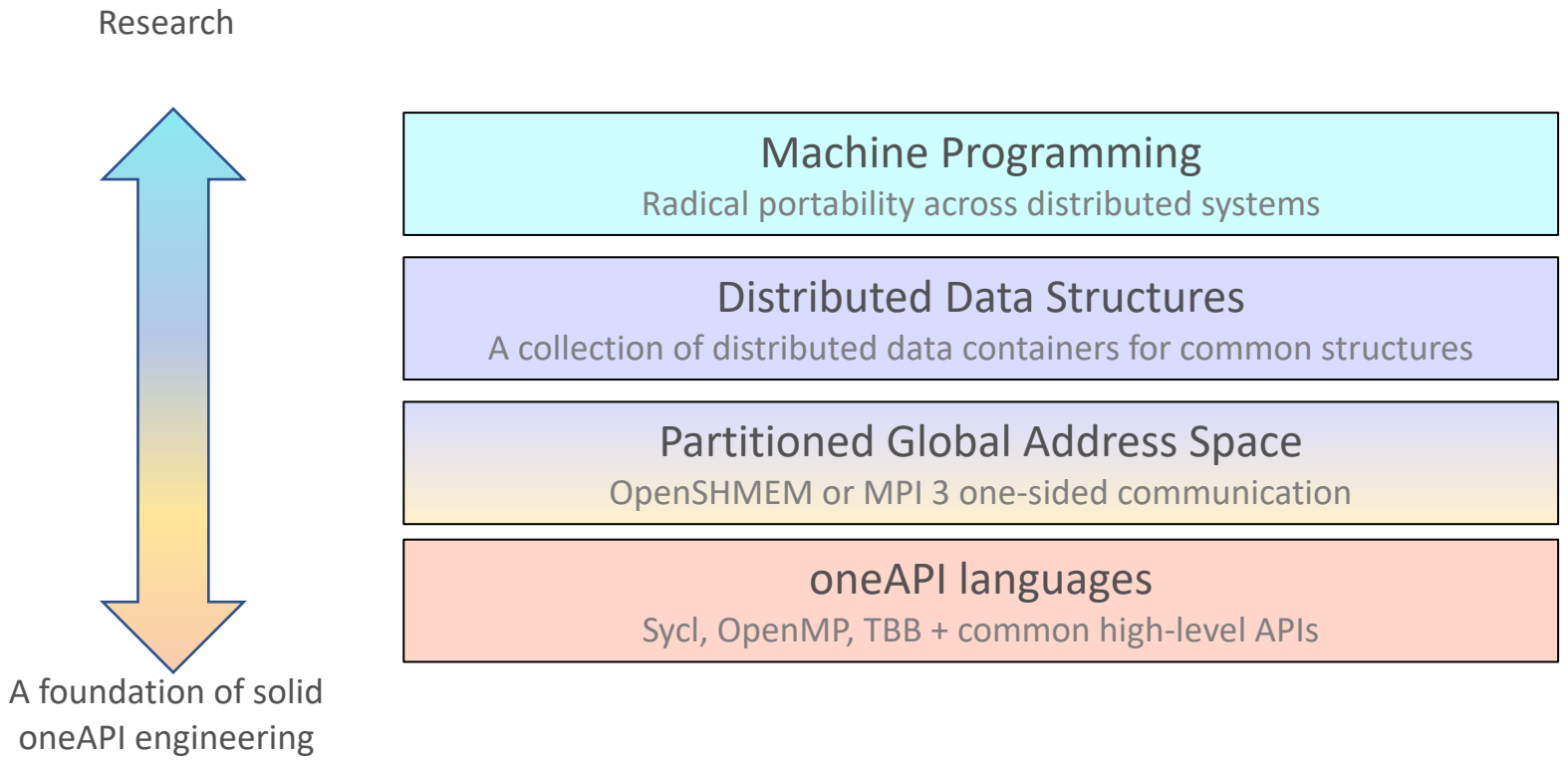
- **MP is the automation of software development**
  - **Intention**: Discover the intent of a programmer
  - **Invention**: Create new algorithms and data structures
  - **Adaptation**: Evolve in a changing hardware/software world

Summarized ~90 works.

Key efforts by Berkeley, Google, Microsoft, MIT, Stanford, UW and others.

oneAPI: A bridge to our heterogeneous/Distributed Future

My vision for how we bring oneAPI into a future dominated by power-optimized heterogenous chips organized into distributed systems.



The key to making this work … the programmer is in control and chooses the level of abstraction based on the programming task.

Summary

- Parallel computing is fun … but it can be hard.
- Fortunately, if you stick to the Big-3 and the core patterns of parallel computing for HPC, it's not too overwhelming
  - The big 3: MPI, OpenMP, and "a GPU programming model"
  - Key Patterns: SPMD, loop level parallelism, geometric decomposition, divide and conquer, and SIMT
- Some day we'll automate the hard-parts with Machine Programming, but that may be 10 years!!!!

SCANPY workload details and system configuration

ame	Intel® Xeon® Platinum 8380
Time	Jan 20, 2022
Manufacturer	Intel Corporation
Product Name	Intel® Xeon® Platinum 8380
BIOS Version	SE5C6200.86B.0020.P23.2103261309
OS	Rocky Linux release 8.5 (Green Obsidian)
Kernel	4.18.0-240.22.1.el8_3.crt6.x86_64
Microcode	0xd000270
IRQ Balance	enabled
CPU Model	Intel(R) Xeon(R) Platinum 8380 CPU @ 2.30GHz
Base Frequency	2.3GHz
Maximum Frequency	3.4GHz
All-core Maximum Frequency	2.5GHz
CPU(s)	40
Thread(s) per Core	2
Core(s) per Socket	40

Socket(s)	1
NUMA Node(s)	1
Prefetchers	
Turbo	Enabled
PPIN(s)	
Power & Perf Policy	Performance
TDP	270 watts
Frequency Driver	
Frequency Governer	Performance
Frequency (MHz)	
Max C-State	
Installed	Intel® Xeon® Platinum 8380 40c D1 DDR4 16*16GB@3200MHz - Mellanox HDR
Huge Pages Size	2048 kB
Transparent Huge Pages	Always
Automatic NUMA Balancing	Enabled

- The following was done to optimize the SCANPY benchmark
  - Data preprocessing - used warm file cache and multi-threaded using Numba JIT
  - PCA, K-means, KNN – Used the Intel extension for scikit-learn.
  - t-SNE - Used optimized version from Intel’s oneDAL Library.
  - Parallelized quadtree building, sorting and summarization steps using Morton codes.
  - UMAP - optimized the UMAP code using AVX512/AVX2. Used MKL for eigenvalue computation.
  - Louvain and Leiden algorithms – collaborated with Katana Graph to get well optimized versions and integrated them into SCANPY.

Backup ... and a bit of extra content

- The future of parallel programming
- The Jacobi solver case study
- Writing functions to call from inside a kernel

Our running example: Jacobi solver

- An iterative method to solve a system of linear equations
  - Given a matrix A and a vector b find the vector x such that Ax=b
- The basic algorithm:
  - Write A as a lower triangular (L), upper triangular (U) and diagonal matrix

    $Ax = (L+D+U)x = b$
  - Carry out multiplications and rearrange

    $Dx=b-(L+U)x \rightarrow x = (b-(L+U)x)/D$
  - Iteratively compute a new x using the x from the previous iteration

    $X_{new} = (b-(L+U)x_{old})/D$
- Advantage: we can easily test if the answer is correct by multiplying our final x by A and comparing to b
- Disadvantage: It takes many iterations and only works for diagonally dominant matrices

Jacobi Solver

Iteratively update xnew until the value stabilizes (i.e. change less than a preset TOL)

```
<<< allocate and initialize the matrix A >>>
<<< and vectors x1, x2 and b             >>>

while((conv > TOL) && (iters<MAX_ITERS))
  {
    iters++;

    for (i=0; i<Ndim; i++){
        xnew[i] = (TYPE) 0.0;
        for (j=0; j<Ndim;j++){
            if(i!=j)
              xnew[i]+= A[i*Ndim + j]*xold[j];
        }
        xnew[i] = (b[i]-xnew[i])/A[i*Ndim+i];
    }
```

```
    // test convergence
    conv = 0.0;
    for (i=0; i<Ndim; i++){
        tmp  = xnew[i]-xold[i];
        conv += tmp*tmp;
    }
    conv = sqrt((double)conv);

    // swap pointers for next
    // iteration
    TYPE* tmp = xold;
    xold = xnew;
    xnew = tmp;

} // end while loop
```

Jacobi Solver (Parallel Target/loop, 1/2)

```
 while((conv > TOL) && (iters<MAX_ITERS))
   {
     iters++;
#pragma omp target map(tofrom:xnew[0:Ndim],xold[0:Ndim]) \
                   map(to:A[0:Ndim*Ndim], b[0:Ndim])
#pragma omp loop
for (i=0; i<Ndim; i++){
        xnew[i] = (TYPE) 0.0;
        for (j=0; j<Ndim;j++){
            if(i!=j)
              xnew[i]+= A[i*Ndim + j]*xold[j];
        }
        xnew[i] = (b[i]-xnew[i])/A[i*Ndim+i];
     }
```

Jacobi Solver (Parallel Target/loop, 2/2)

```
    //
    // test convergence
    //
    conv = 0.0;
#pragma omp target map(to:xnew[0:Ndim],xold[0:Ndim]) \
                   map(tofrom:conv)
#pragma omp loop private(i,tmp) reduction(+:conv)
for (i=0; i<Ndim; i++){
        tmp  = xnew[i]-xold[i];
        conv += tmp*tmp;
    }
    conv = sqrt((double)conv);
   TYPE* tmp = xold;
   xold = xnew;
   xnew = tmp;
} // end while loop
```

This worked but the performance was awful. Why?

System	Implementation	Ndim = 4096
NVIDA® K20X™ GPU	Target dir per loop	131.94 secs

Cray® XC40™ Supercomputer running Cray® Compiling Environment 8.5.3.
Intel® Xeon ® CPU E5-2697 v2 @ 2.70GHz with 32 GB DDR3. NVIDIA® Tesla® K20X, 6GB.

Data movement dominates!!!

```
while((conv > TOLERANCE) && (iters<MAX_ITERS))
  { iters++;
    xnew = iters % s ? x2 : x1;
    xold   = iters % s ? x1 : x2;

    #pragma omp target map(tofrom:xnew[0:Ndim],xold[0:Ndim]) \
                       map(to:A[0:Ndim*Ndim], b[0:Ndim] )
     #pragma omp loop private(i,j)
     for (i=0; i<Ndim; i++){
        xnew[i] = (TYPE) 0.0;
        for (j=0; j<Ndim;j++){
            if(i!=j)
              xnew[i]+= A[i*Ndim + j]*xold[j];
        }
        xnew[i] = (b[i]-xnew[i])/A[i*Ndim+i];
     }
// test convergence
    conv = 0.0;
    #pragma omp target map(to:xnew[0:Ndim],xold[0:Ndim]) \
                                map(tofrom:conv)
     #pragma loop reduction(+:conv)
     for (i=0; i<Ndim; i++){
        tmp  = xnew[i]-xold[i];
        conv += tmp*tmp;
     }
    conv = sqrt((double)conv);
  }
```

Typically over 4000 iterations!

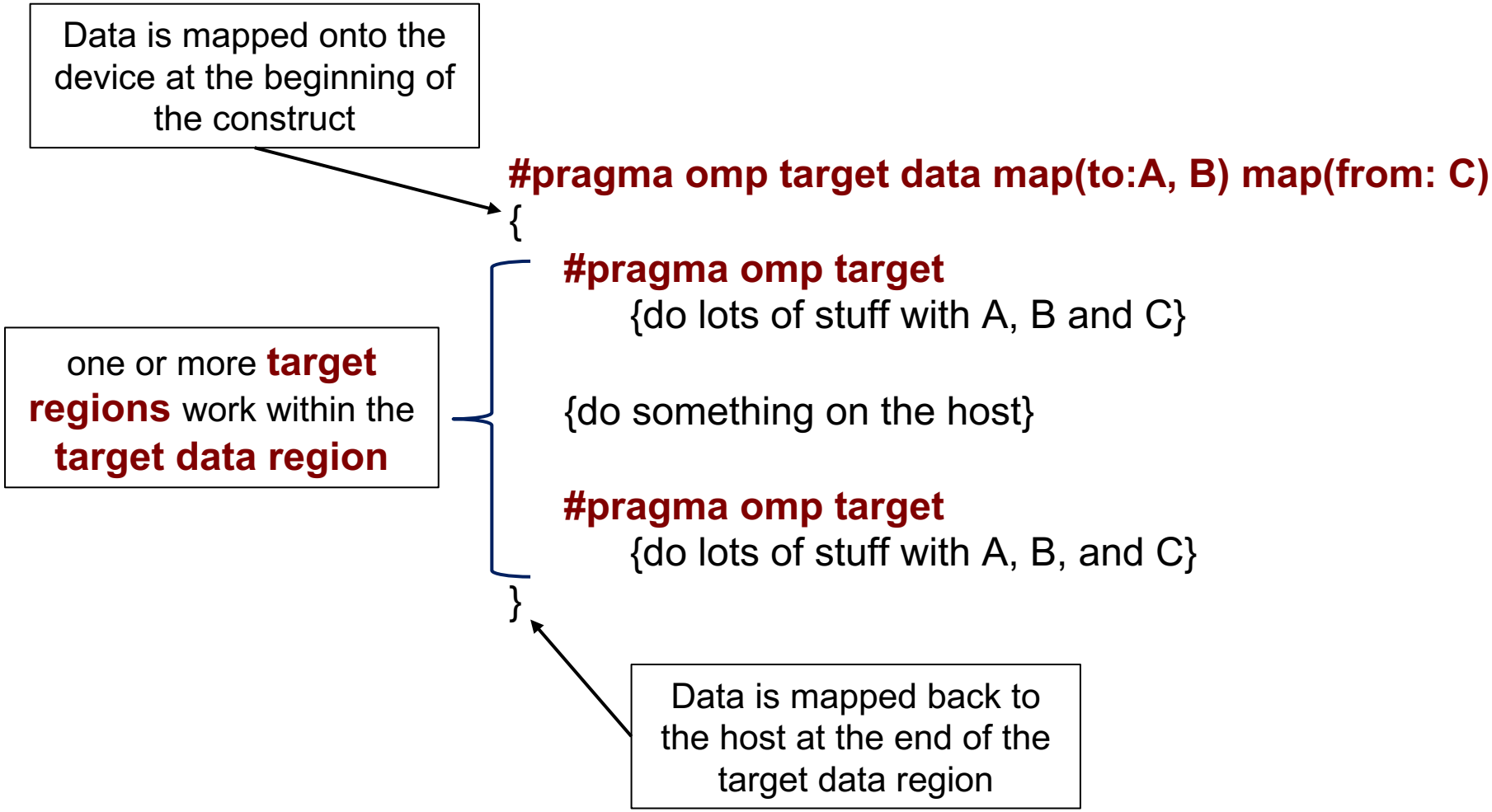
For each iteration, copy to device $(3*Ndim+Ndim^2)*sizeof(TYPE)$ bytes

For each iteration, copy from device $2*Ndim*sizeof(TYPE)$ bytes

For each iteration, copy to device $2*Ndim*sizeof(TYPE)$ bytes

Target data directive

- The **target data** construct creates a target data region
  … use **map** clauses for explicit data management



Jacobi Solver (Par Target Data, 1/2)

```
#pragma omp target data map(tofrom:xold[0:Ndim],xnew[0:Ndim]) \
                        map(to:A[0:Ndim*Ndim], b[0:Ndim] ,Ndim)
while((conv > TOL) && (iters<MAX_ITERS))
  {  iters++;

#pragma omp target
#pragma omp loop private(j) firstprivate(xnew,xold)
    for (i=0; i<Ndim; i++){
        xnew[i] = (TYPE) 0.0;
        for (j=0; j<Ndim;j++){
            if(i!=j)
              xnew[i]+= A[i*Ndim + j]*xold[j];
        }
        xnew[i] = (b[i]-xnew[i])/A[i*Ndim+i];
    }
```

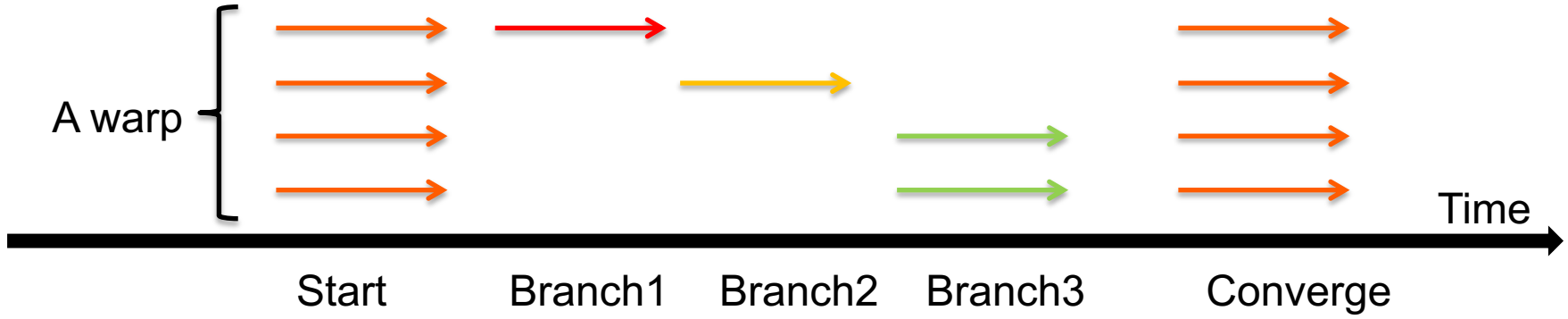
Jacobi Solver (Par Target Data, 2/2)

```
// test convergence
conv = 0.0;
#pragma omp target map(tofrom: conv)
#pragma omp loop private(tmp) firstprivate(xnew,xold)  reduction(+:conv)

    for (i=0; i<Ndim; i++){
        tmp  = xnew[i]-xold[i];
        conv += tmp*tmp;
    }
// end target region
 conv = sqrt((double)conv);

   TYPE* tmp = xold;
   xold = xnew;
   xnew = tmp;
} // end while loop
```

System	Implementation	Ndim = 4096
NVIDA® K20X™ GPU	Target dir per loop	131.94 secs
	Above plus target data region	18.37 secs

Single Instruction Multiple Data

- Individual work-items of a warp start together at the same program address
- Each work-item has its own instruction address counter and register state
  - Each work-item is free to branch and execute independently
  - Supports the SPMD pattern.
- Branch behavior
  - Each branch will be executed serially
  - Work-items not following the current branch will be disabled



Branching

Conditional execution

```
// Only evaluate expression
// if condition is met
if (a > b)
{
  acc += (a - b*c);
}
```

Selection and masking

```
// Always evaluate expression
// and mask result
temp = (a - b*c);
mask = (a > b ? 1.f : 0.f);
acc += (mask * temp);
```

Coalescence

- Coalesce - to combine into one
- Coalesced memory accesses are key for high bandwidth
- Simply, it means, if thread *i* accesses memory location *n* then thread *i+1* accesses memory location *n+1*
- In practice, it's not quite as strict…

```
for (int id = 0; id < size; id++)
{
  // ideal
     float val1 = memA[id];

  // still pretty good
     const int c = 3;
     float val2 = memA[id + c];

  // stride size is not so good
     float val3 = memA[c*id];

  // terrible
     const int loc =
       some_strange_func(id);

     float val4 = memA[loc];
}
```

Jacobi Solver (Target Data/branchless/coalesced mem, 1/2)

```
#pragma omp target data map(tofrom:x1[0:Ndim],x2[0:Ndim]) \
                        map(to:A[0:Ndim*Ndim], b[0:Ndim] ,Ndim)
while((conv > TOL) && (iters<MAX_ITERS))
  {  iters++;
#pragma omp target
     #pragma omp loop private(j)
    for (i=0; i<Ndim; i++){
       xnew[i] = (TYPE) 0.0;
       for (j=0; j<Ndim;j++){
            xnew[i]+= (A[j*Ndim + i]*xold[j])*((TYPE)(i != j));
       }
       xnew[i] = (b[i]-xnew[i])/A[i*Ndim+i];
    }
```

We replaced the original code with a poor memory access pattern

```
xnew[i]+= (A[i*Ndim + j]*xold[j])
```

With the more efficient

```
xnew[i]+= (A[j*Ndim + i]*xold[j])
```

Jacobi Solver (Target Data/branchless/coalesced mem, 2/2)

```
      //
      // test convergence
      conv = 0.0;
#pragma omp target map(tofrom: conv)
 #pragma omp loop private(tmp) reduction(+:conv)
      for (i=0; i<Ndim; i++){
          tmp  = xnew[i]-xold[i];
          conv += tmp*tmp;
      }
conv = sqrt((double)conv);
    TYPE* tmp = xold;
    xold = xnew;
    xnew = tmp;
} // end while loop
```

System	Implementation	Ndim = 4096
NVIDA® K20X™ GPU	Target dir per loop	131.94 secs
	Above plus target data region	18.37 secs
	Above plus reduced branching	13.74 secs
	Above plus improved mem access	7.64 secs

Cray® XC40™ Supercomputer running Cray® Compiling Environment 8.5.3.
Intel® Xeon ® CPU E5-2697 v2 @ 2.70GHz with 32 GB DDR3. NVIDIA® Tesla® K20X, 6GB.

A more complicated example:
Jacobi iteration: OpenACC (GPU)

```
#pragma acc data copy(A), create(Anew)
while (err>tol && iter < iter_max){
   err = 0.0;
   #pragma acc parallel loop reduction(max:err)
   for(int j=1; j< n-1; j++){
      for(int i=1; i<M-1; i++){
         Anew[j][i] = 0.25* (A[j][i+1] + A[j][i-1]+
                             A[j-1][i] + A[j+1][i]);
         err = max(err,abs(Anew[j][i] - A[j][i]));
       }
    }
    #pragma acc parallel loop
    for(int j=1; j< n-1; j++){
      for(int i=1; i<M-1; i++){
         A[j][i] = Anew[j]i];
       }
    }
    iter ++;
}
```

Create a data region on the GPU. Copy A once onto the GPU, and create Anew on the device (no copy from host)

Copy A back out to host … but only once

Source: based on Mark Harris of NVIDIA®, “Getting Started with OpenACC”, GPU technology Conf., 2012

A more complicated example:

Jacobi iteration: OpenMP target directives

```
#pragma omp target data map(A) map(alloc:Anew)
while (err>tol && iter < iter_max){
   err = 0.0;
   #pragma target
   #pragma omp teams loop reduction(max:err)
   for(int j=1; j< n-1; j++){
      for(int i=1; i<M-1; i++){
         Anew[j][i] = 0.25* (A[j][i+1] + A[j][i-1]+
                             A[j-1][i] + A[j+1][i]);
         err = max(err,abs(Anew[j][i] - A[j][i]));
       }
    }
    #pragma omp target
    #pragma omp teams loop
    for(int j=1; j< n-1; j++){
      for(int i=1; i<M-1; i++){
         A[j][i] = Anew[j]i];
       }
    }
    iter ++;
}
```

Create a data region on the GPU. Map A and Anew onto the target device

Copy A back out to host … but only once

Backup ... and a bit of extra content

- The future of parallel programming
- The Jacobi solver case study
- Writing functions to call from inside a kernel

Defining a function to be called from inside a kernel

Tell OpenMP to compile this function for the GPU (and the CPU)

Call inside a target region, and the GPU version is called.

Call on the host, and a CPU version is called

```
#include mm_utils.h

#pragma omp declare target
void ddot(double *C, double *A, double *B, int i, int j, int Mdim, int Pdim){
   for(int k=0;k<Pdim;k++){
      /* C(i,j) = sum(over k) A(i,k) * B(k,j) */
      *(C+(i*Mdim+j)) += *(A+(i*Pdim+k)) *  *(B+(k*Mdim+j));
   }
}
#pragma omp end declare target


void mm_gpu(int Ndim, int Mdim, int Pdim, TYPE *A, TYPE *B, TYPE *C){
  int i, j, k;

#pragma omp target teams map(tofrom:C[0:Ndim*Mdim]) map(to:B[0:Pdim*Mdim],A[0:Ndim*Pdim])
#pragma omp loop  collapse(2)
  for (i=0; i<Ndim; i++){
     for (j=0; j<Mdim; j++){
        ddot(C, A, B, i, j, Mdim, Pdim);

     }
```

This is in my file mm_gpu.c

ncu –set=detailed ./a.out

```
==PROF== Connected to process 3522427
(/home/tgmattso/ParProgForPhys/OMP_GPU_Exercises/Solutions/a.out)
==PROF== Profiling "nvkernel_main_F1L28_3" - 0: 0%....50%....100% - 11 passes
==PROF== Disconnected from process 3522427
 vectors added with 0 errors
[3522427] a.out@127.0.0.1
  nvkernel_main_F1L28_3 (108, 1, 1)x(128, 1, 1), Context 1, Stream 16, Device
0, CC 8.0
    Section: GPU Speed Of Light Throughput
    ---------------------- ------------ ------------
    Metric Name              Metric Unit Metric Value
    ---------------------- ------------ ------------
    DRAM Frequency          cycle/nsecond         1.21
    SM Frequency            cycle/nsecond         1.10
    Elapsed Cycles                  cycle    9,206,395
    Memory Throughput                   %         1.92
    DRAM Throughput                     %         0.01
    Duration                       msecond         8.35
    L1/TEX Cache Throughput             %         1.68
    L2 Cache Throughput                 %         2.03
    SM Active Cycles                cycle 9,153,430.62
    Compute (SM) Throughput             %         1.74
    ---------------------- ------------ ------------
    OPT   This kernel grid is too small to fill the available resources on this
device, resulting in only 0.1 full waves across all SMs. Look at Launch Statistics
for more details.


    Section: Launch Statistics
    -------------------------------- --------------- ---------------
    Metric Name                          Metric Unit    Metric Value
    -------------------------------- --------------- ---------------
    Block Size                                                   128
    Function Cache Configuration                      CachePreferNone
    Grid Size                                                    108
    Registers Per Thread                register/thread              50
    Shared Memory Configuration Size              Kbyte           65.54
    Driver Shared Memory Per Block        Kbyte/block            1.02
    Dynamic Shared Memory Per Block       Kbyte/block            1.63
    Static Shared Memory Per Block         byte/block               0
    Threads                                     thread          13,824
    Waves Per SM                                                 0.11
    -------------------------------- --------------- ---------------
```

cc –mp=gpu vadd.c

```
    OPT   If you execute __syncthreads() to synchronize the
threads of a block, it is recommended to have more than the
achieved 1 blocks per multiprocessor. This way, blocks that
aren't waiting for __syncthreads() can keep th3e hardware
busy.


    Section: Occupancy
    ------------------------------- ----------- ------------
    Metric Name                     Metric Unit Metric Value
    ------------------------------- ----------- ------------
    Block Limit SM                        block           32
    Block Limit Registers                 block            9
    Block Limit Shared Mem                block           24
    Block Limit Warps                     block           16
    Theoretical Active Warps per SM        warp           36
    Theoretical Occupancy                     %        56.25
    Achieved Occupancy                        %         6.25
    Achieved Active Warps Per SM           warp         4.00
    ------------------------------- ----------- ------------


    OPT   Estimated Speedup:
88.89%

          This kernel's theoretical occupancy (56.2%) is limited
by the number of required registers. The difference between
calculated theoretical (56.2%) and measured achieved occupancy
(6.2%) can be the result of warp scheduling overheads or
workload imbalances during the kernel execution. Load imbalances
can occur between warps within a block as well as across blocks
of the same kernel. See
the CUDA Best Practices Guide
(https://docs.nvidia.com/cuda/cuda-c-best-practices-
guide/index.html#occupancy) for more details on optimizing
occupancy.
```