



The Parallel Programming World Beyond OpenMP

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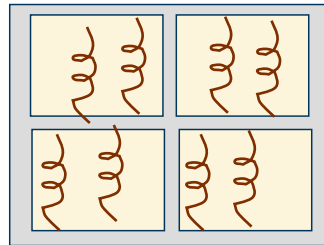
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just to make sure we don't miss anything important.

I have a really great job!!!!

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



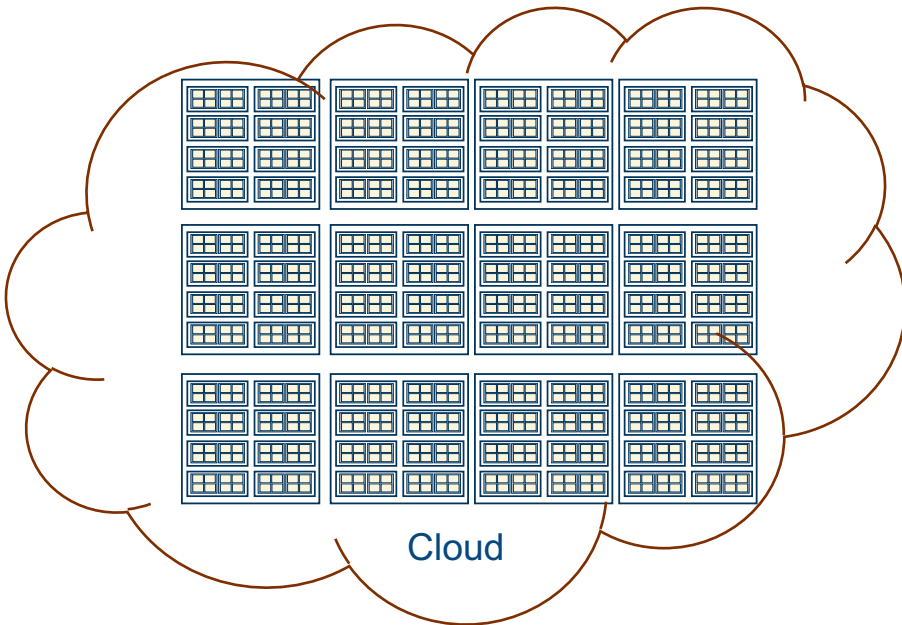
CPU



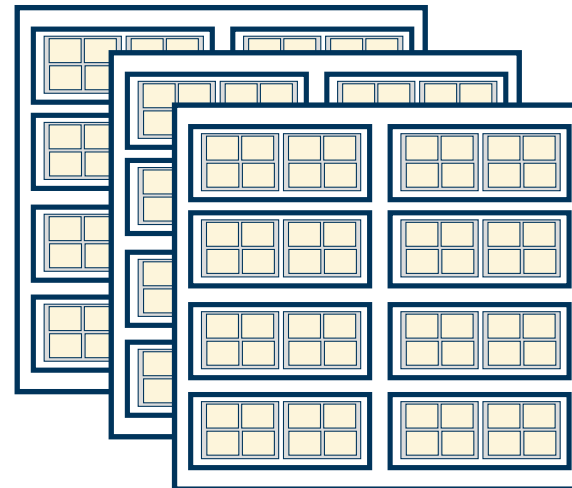
SIMD/Vector



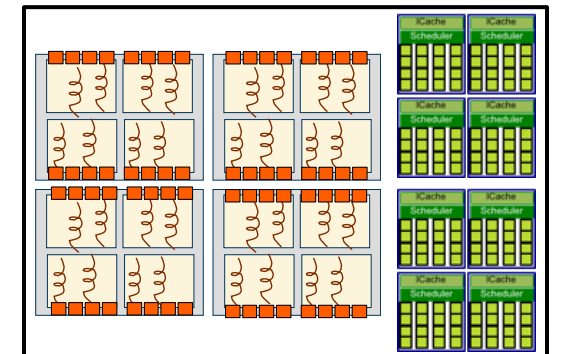
GPU



Cloud



Cluster



Heterogeneous node

The Big Three

- 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)
- 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.

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

The Big Three

If you don't know MPI, you really aren't an HPC programmer!



- In HPC, 3 programming environments dominate ... covering the major classes of hardware.
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 - **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)
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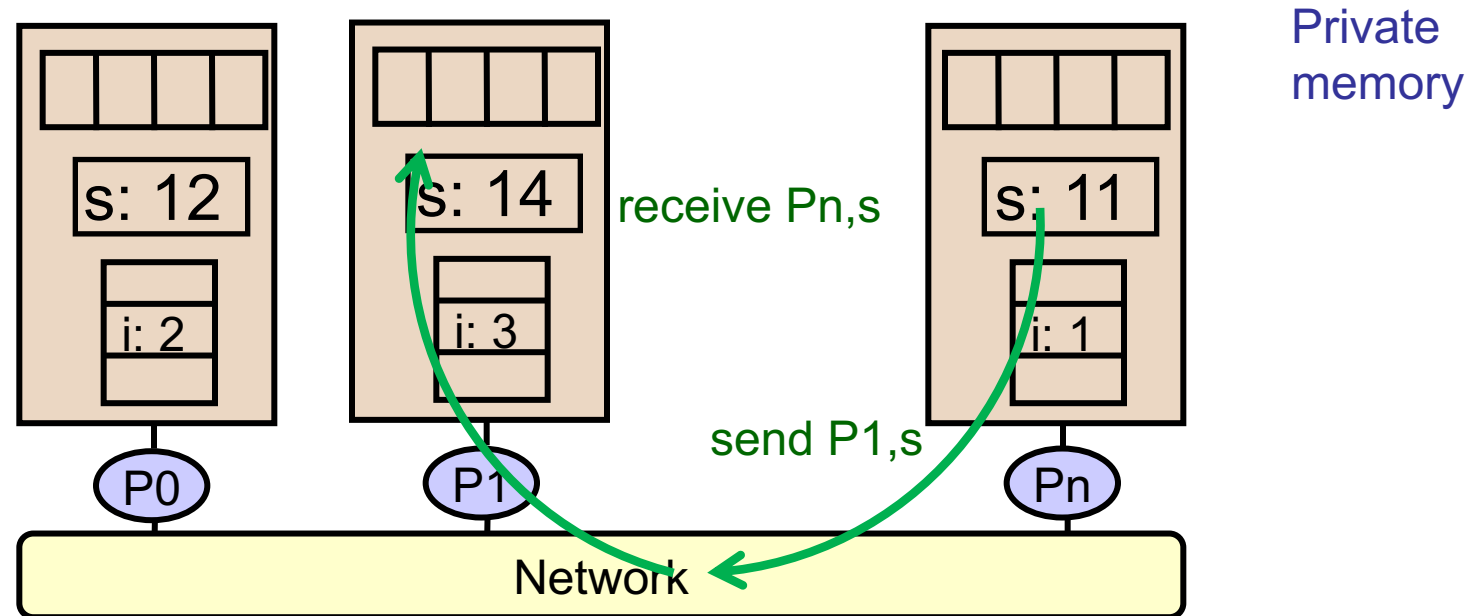
Parallel API's: MPI ... the Message Passing Interface

MPI: An API for Writing Clustered Applications

- A library of routines to coordinate the execution of multiple processes.
- Provides point to point and collective communication in Fortran, C and C++
- Unifies last 25+ years of cluster computing and MPP practice

Programming Model: Message Passing

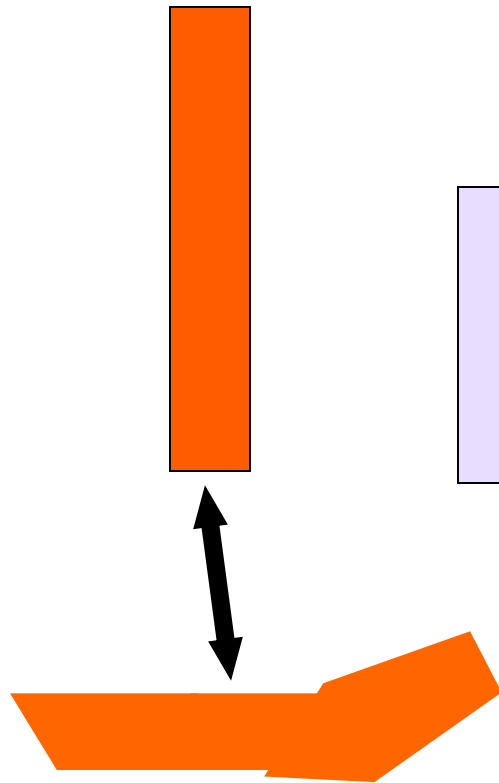
- Program consists of a collection of **named** processes.
 - Number of processes almost always fixed at program startup time
 - Local address space per node -- NO physically shared memory.
 - Logically shared data is partitioned over local processes.
- Processes communicate by explicit send/receive pairs
 - Coordination is implicit in every communication event.
 - MPI (Message Passing Interface) is the most commonly used SW



How do people use MPI?

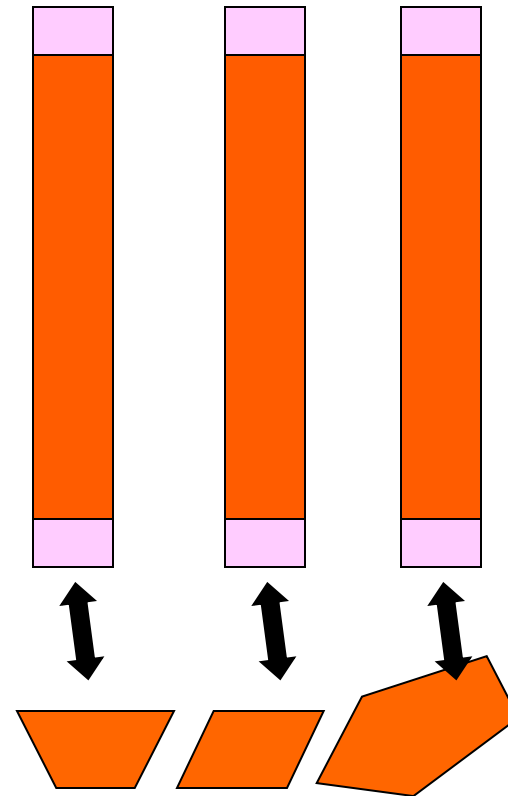
The SPMD Design Pattern

A sequential program
working on a data set



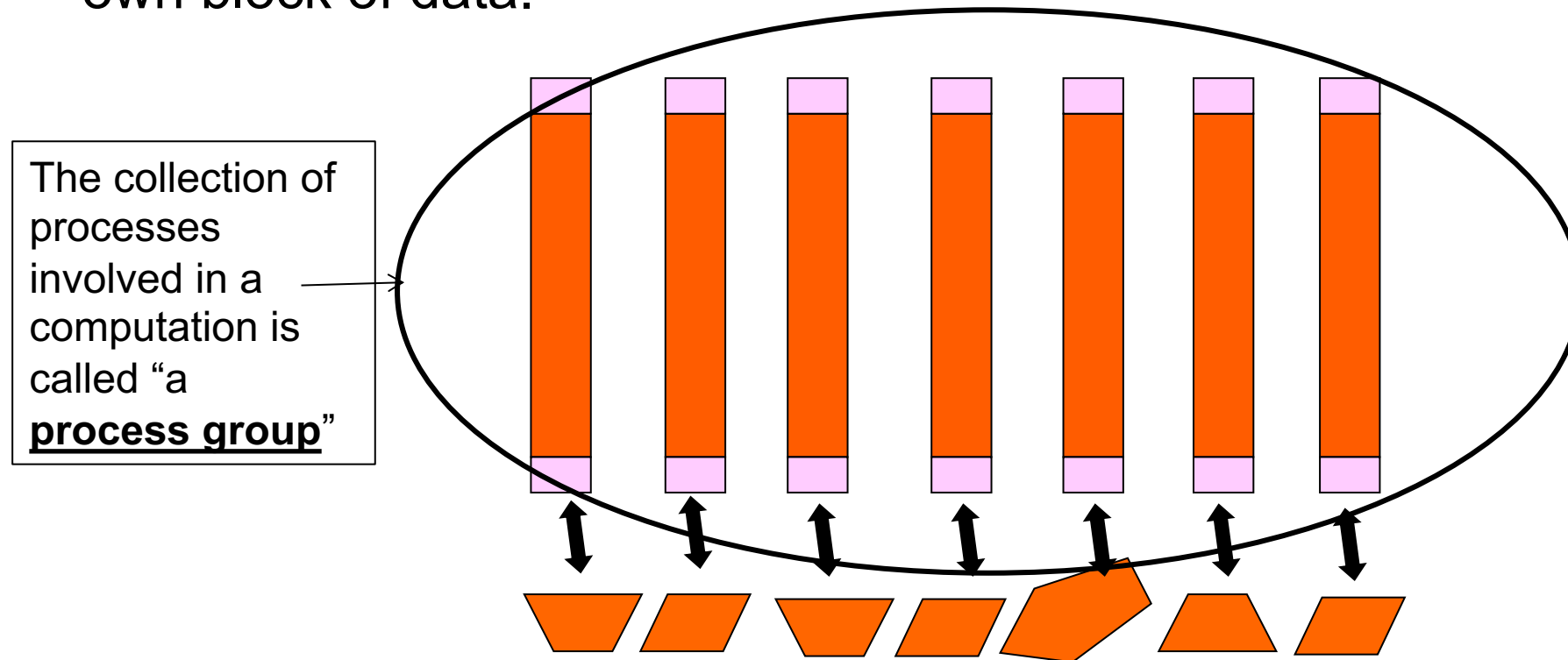
Replicate the program.
Add glue code
Break up the data

- A single program working on a decomposed data set.
- Use Node ID and numb of nodes to split up work between processes
- Coordination by passing messages.



An MPI program at runtime

- Typically, when you run an MPI program, multiple processes running the same program are launched ... working on their own block of data.



MPI functions work within a "**context**": MPI actions occurring in different contexts, even if they share a process group, cannot interfere with each other.

MPI Hello World

```
#include <stdio.h>
#include <mpi.h>
int main (int argc, char **argv){
    int rank, size;
    MPI_Init (&argc, &argv);
    MPI_Comm_rank (MPI_COMM_WORLD, &rank);
    MPI_Comm_size (MPI_COMM_WORLD, &size);
    printf( "Hello from process %d of %d\n",
           rank, size );

    MPI_Finalize();
    return 0;
}
```

Initializing and finalizing MPI

```
int MPI_Init (int* argc, char* argv[])
```

- Initializes the MPI library ... called before any other MPI functions.
- argc and argv are the command line args passed from main()

```
#include <stdio.h>
```

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

```
int main (int argc, char **argv){
```

```
    int rank, size;
```

```
    MPI_Init (&argc, &argv);
```

```
    MPI_Comm_rank (MPI_COMM_WORLD, &rank);
```

```
    MPI_Comm_size (MPI_COMM_WORLD, &size);
```

```
    printf( "Hello from process %d of %d\n",  
           rank, size );
```

```
    MPI_Finalize();
```

```
    return 0;
```

```
}
```

```
int MPI_Finalize (void)
```

- Frees memory allocated by the MPI library ... close every MPI program with a call to MPI_Finalize

How many processes are involved?

```
int MPI_Comm_size (MPI_Comm comm, int* size)
```

- `MPI_Comm`, an *opaque data type* called a *communicator*. Default context: `MPI_COMM_WORLD` (all processes)
- `MPI_Comm_size` returns the number of processes in the process group associated with the communicator

```
#include
```

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

```
int main (int argc, char **argv){
```

```
    int rank, size;
```

```
    MPI_Init (&argc, &argv);
```

```
    MPI_Comm_rank (MPI_COMM_WORLD, &rank);
```

```
    MPI_Comm_size (MPI_COMM_WORLD, &size);
```

```
    printf( "Hello from process %d of %d\n",  
            rank, size );
```

```
    MPI_Finalize();
```

```
    return 0;
```

```
}
```

Communicators consist of two parts, a **context** and a **process group**.

The communicator lets one control how groups of messages interact.

Communicators support modular SW ... i.e. I can give a library module its own communicator and know that its messages can't collide with messages originating from outside the module

Which process “am I” (the rank)

```
int MPI_Comm_rank (MPI_Comm comm, int* rank)
```

- `MPI_Comm`, an *opaque data type*, a communicator. Default context: `MPI_COMM_WORLD` (all processes)
- `MPI_Comm_rank` An integer ranging from 0 to “(num of procs)-1”

```
#include <mpi.h>
int main (int argc, char **argv){
    int rank, size;
    MPI_Init (&argc, &argv);
    MPI_Comm_rank (MPI_COMM_WORLD, &rank);
    MPI_Comm_size (MPI_COMM_WORLD, &size);
    printf( "Hello from process %d of %d\n",
            rank, size );

    MPI_Finalize();
    return 0;
}
```

Note that other than `init()` and `finalize()`, every MPI function has a communicator.

This makes sense .. You need a context and group of processes that the MPI functions impact ... and those come from the communicator.

Running the program

```
#include <stdio.h>
#include <mpi.h>
int main (int argc, char **argv){
    int rank, size;
    MPI_Init (&argc, &argv);
    MPI_Comm_rank (MPI_COMM_WORLD, &rank);
    MPI_Comm_size (MPI_COMM_WORLD, &size);
    printf( "Hello from process %d of %d\n",
           rank, size );

    MPI_Finalize();
    return 0;
}
```

- On a 4 node cluster, I'd run this program (hello) as:
 - > mpiexec -np 4 -hostfile hostf hello
- Where "hostf" is a file with the names of the cluster nodes, one to a line.
- What would this program would output?

Running the program

```
#include <stdio.h>
#include <mpi.h>
int main (int argc, char **argv){
    int rank, size;
    MPI_Init (&argc, &argv);
    MPI_Comm_rank (MPI_COMM_WORLD, &rank);
    MPI_Comm_size (MPI_COMM_WORLD, &size);
    printf( "Hello from process %d of %d\n",
           rank, size );

    MPI_Finalize();
    return 0;
}
```

- On a 4 node cluster, I'd run this program (hello) as:
 > mpiexec -np 4 -hostfile hostf hello
 Hello from process 1 of 4
 Hello from process 2 of 4
 Hello from process 0 of 4
 Hello from process 3 of 4
- Where "hostf" is a file with the names of the cluster nodes, one to a line.

Bulk Synchronous Programming:

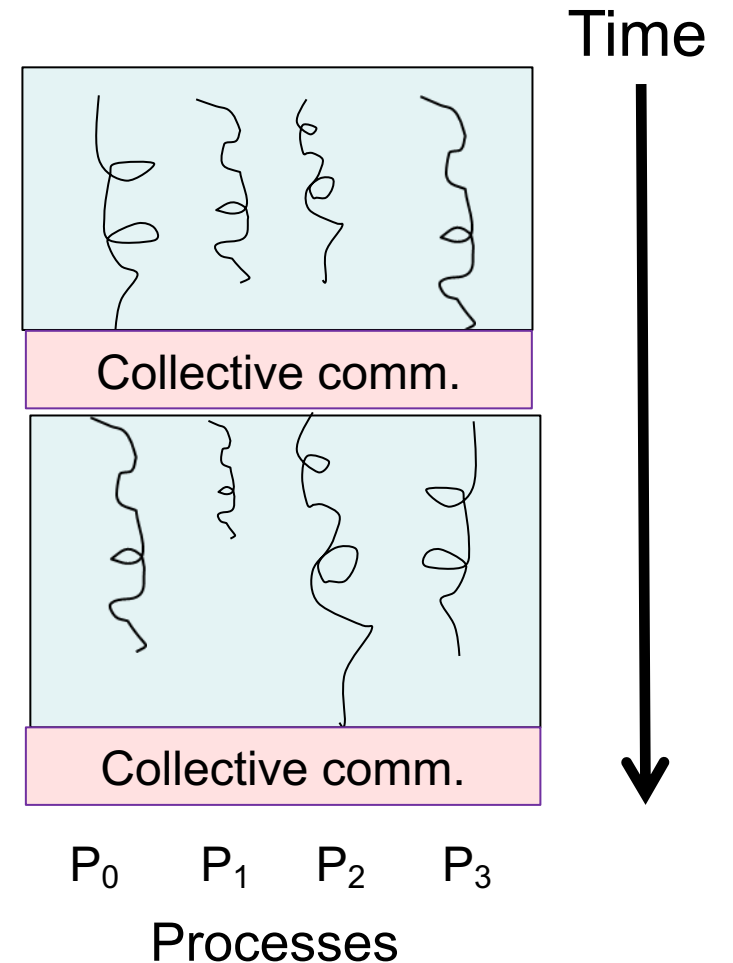
A common design pattern used with MPI Programs

- Many MPI applications have few (if any) sends and receives.

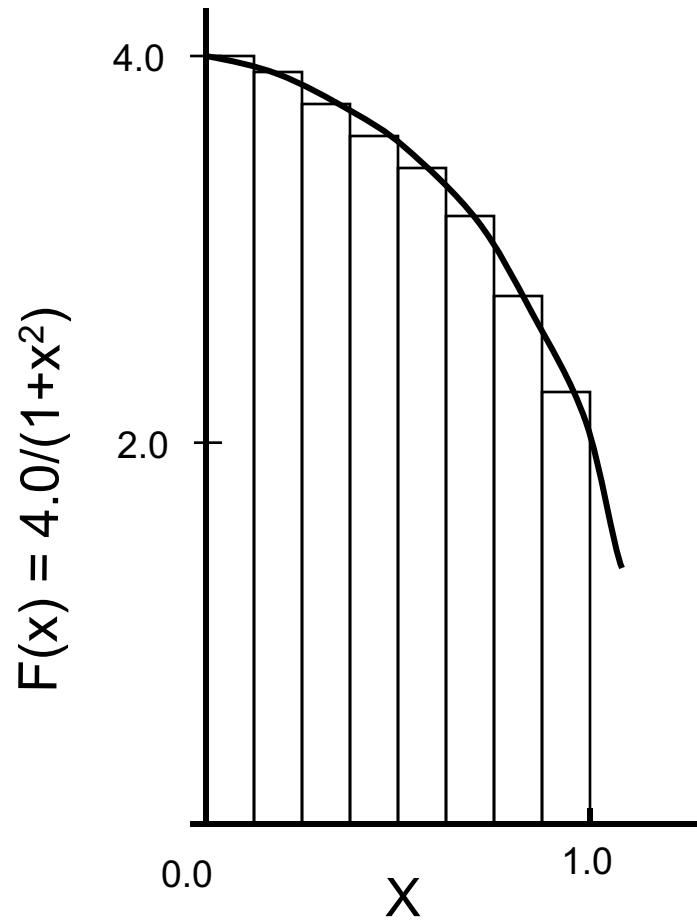
They use the following very common pattern:

- Use the Single Program Multiple Data pattern
- Each process maintains a local view of the global data
- A problem broken down into phases each of which is composed of two subphases:
 - Compute on local view of data
 - Communicate to update global view on all processes (collective communication).
- Continue phases until complete

This is a subset or the SPMD pattern sometimes referred to as the Bulk Synchronous pattern.



Example Problem: Numerical Integration



Mathematically, we know that:

$$\int_0^1 \frac{4.0}{(1+x^2)} dx = \pi$$

We can approximate the integral as a sum of rectangles:

$$\sum_{i=0}^N F(x_i) \Delta x \approx \pi$$

Where each rectangle has width Δx and height $F(x_i)$ at the middle of interval i .

PI Program: an example

```
static long num_steps = 100000;
double step;
void main ()
{
    int i;    double x, pi, sum = 0.0;

    step = 1.0/(double) num_steps;
    x = 0.5 * step;
    for (i=0;i<= num_steps; i++){
        x+=step;
        sum += 4.0/(1.0+x*x);
    }
    pi = step * sum;
}
```

Pi program in MPI ... using the BSP pattern

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

```
void main (int argc, char *argv[])
```

```
{
```

```
    int i, my_id, numprocs; double x, pi, step, sum = 0.0 ;
```

```
    step = 1.0/(double) num_steps ;
```

```
    MPI_Init(&argc, &argv) ;
```

```
    MPI_Comm_Rank(MPI_COMM_WORLD, &my_id) ;
```

```
    MPI_Comm_Size(MPI_COMM_WORLD, &numprocs) ;
```

```
    my_steps = num_steps/numprocs ;
```

```
    for (i=my_id*my_steps; i<(my_id+1)*my_steps ; i++)
```

```
    {
```

```
        x = (i+0.5)*step;
```


```
        sum += 4.0/(1.0+x*x);
```

```
    }
```

```
    sum *= step ;
```

```
    MPI_Reduce(&sum, &pi, 1, MPI_DOUBLE, MPI_SUM, 0,  
             MPI_COMM_WORLD) ;
```

```
}
```



Sum values in "sum" from
each process and place it
in "pi" on process 0

Reduction

```
int MPI_Reduce (void* sendbuf,  
               void* recvbuf, int count,  
               MPI_Datatype datatype, MPI_Op op,  
               int root, MPI_Comm comm)
```

- **MPI_Reduce** performs specified reduction operation on specified data from all processes in communicator, places result in process “root” only.
- **MPI_Allreduce** places result in all processes (avoid unless necessary)

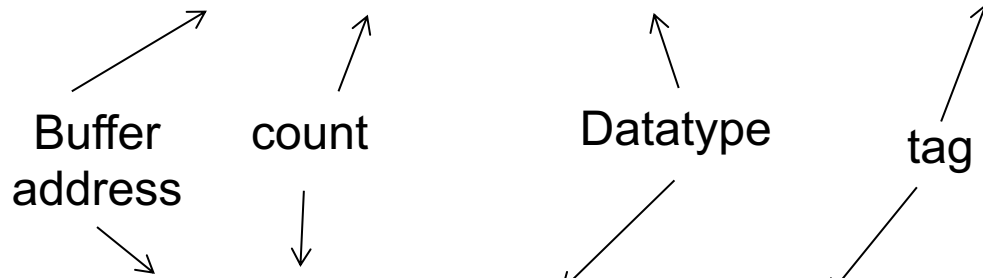
Operation	Function
MPI_SUM	Summation
MPI_PROD	Product
MPI_MIN	Minimum value
MPI_MINLOC	Minimum value and location
MPI_MAX	Maximum value
MPI_MAXLOC	Maximum value and location
MPI_LAND	Logical AND

Operation	Function
MPI_BAND	Bitwise AND
MPI_LOR	Logical OR
MPI_BOR	Bitwise OR
MPI_LXOR	Logical exclusive OR
MPI_BXOR	Bitwise exclusive OR
User-defined	It is possible to define new reduction operations

Sending and receiving messages

- Pass a buffer which holds “count” values of MPI_TYPE
- The data in a message to send or receive is described by a triple:
 - **(address, count, datatype)**
- The receiving process identifies messages with the double :
 - **(source, tag)**
- Where:
 - Source is the rank of the sending process
 - Tag is a user-defined integer to help the receiver keep track of different messages from a single source

MPI_Send (buff, 100, MPI_DOUBLE, Dest, tag, MPI_COMM_WORLD);

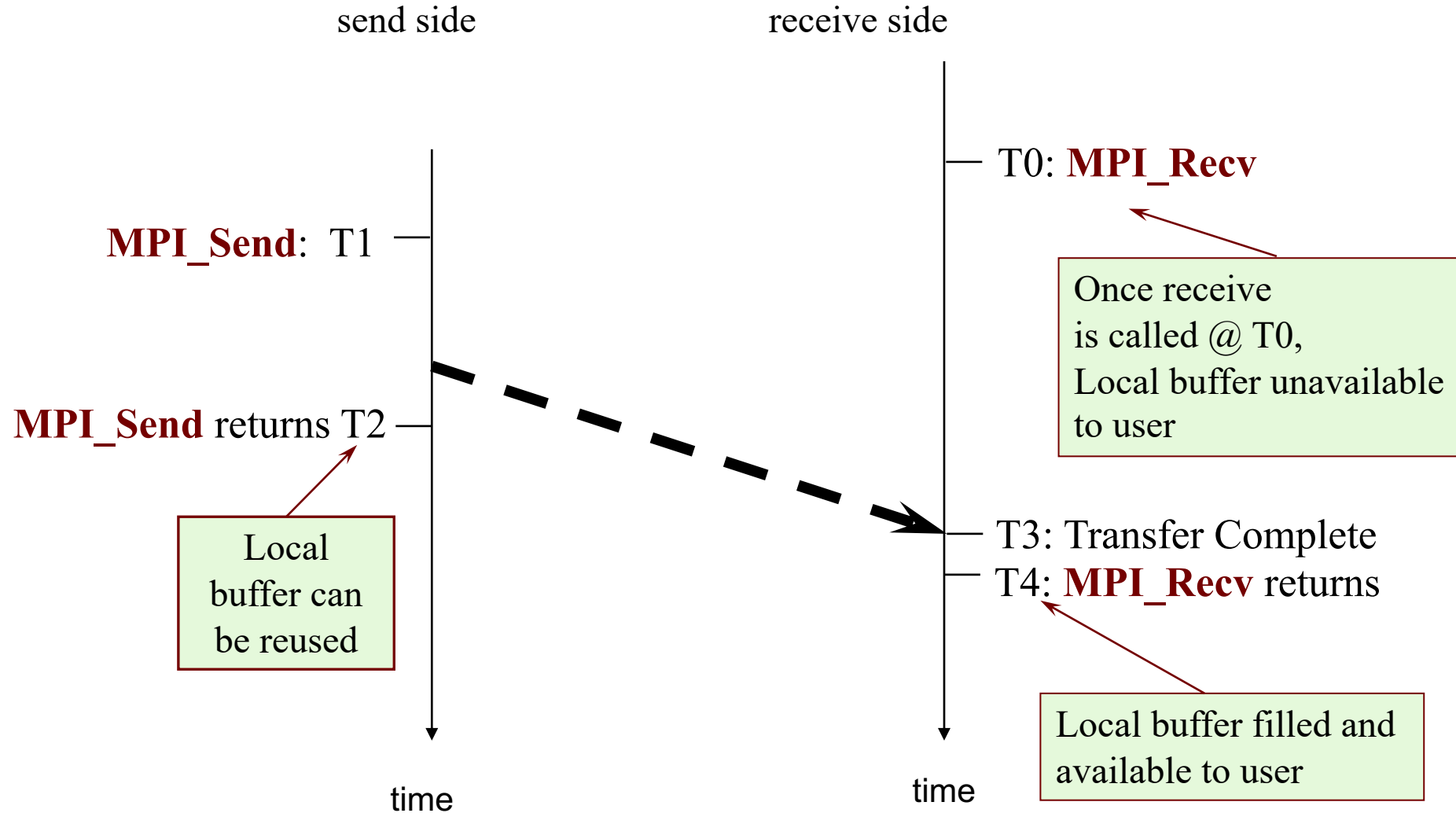


MPI_Recv (buff, 100, MPI_DOUBLE, Src, tag, MPI_COMM_WORLD, &status);

Rank of Source node

Blocking Send-Receive Timing Diagram

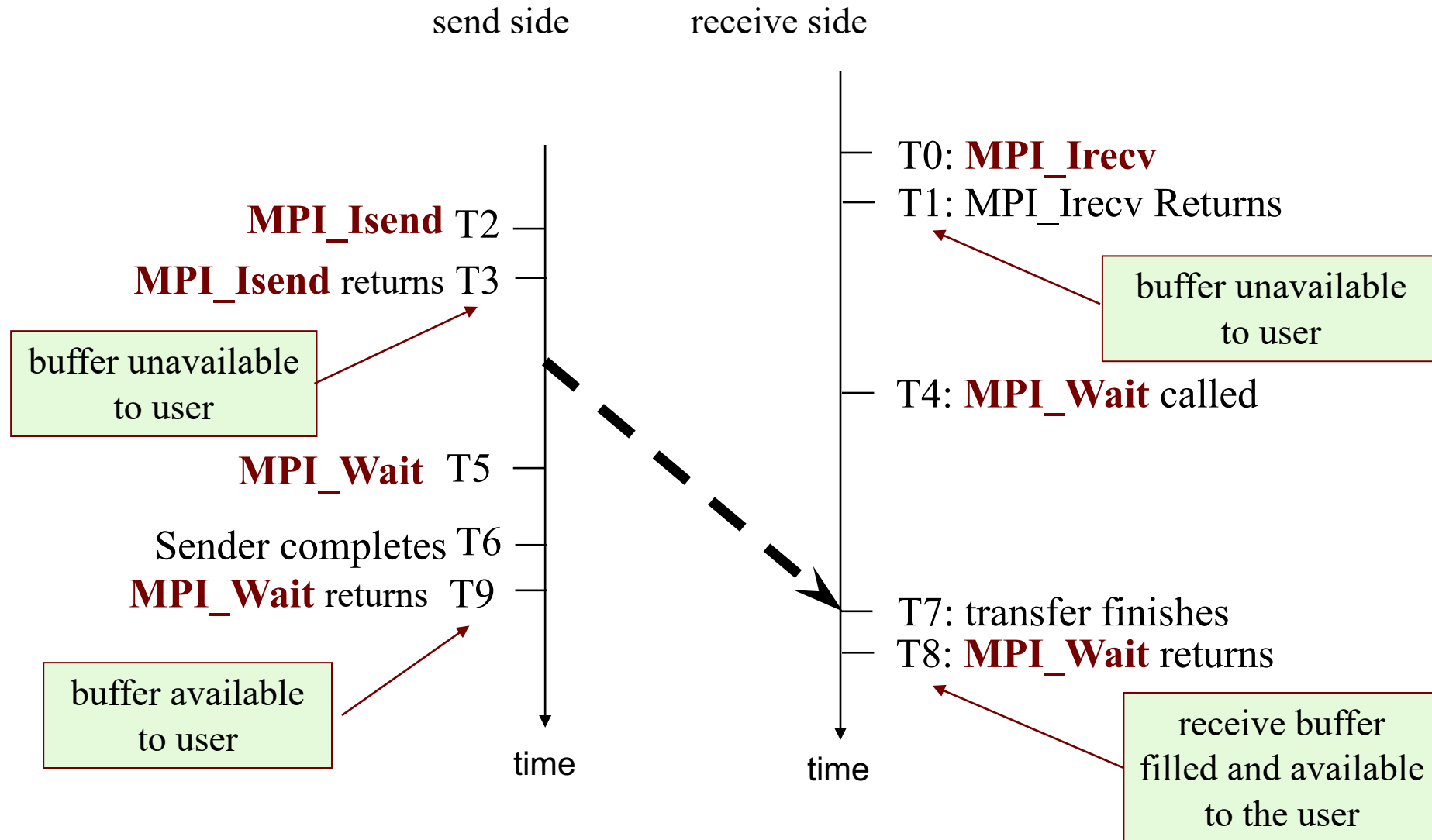
(MPI functions return when local buffer can be used again)



It is important to post the receive before sending, for highest performance.

Non-Blocking Send-Receive Diagram

(MPI functions return immediately)



Example: finite difference methods

- Solve the heat diffusion equation in 1 D:
 - $u(x,t)$ describes the temperature field
 - We set the heat diffusion constant to one
 - Boundary conditions, constant u at endpoints.

$$\frac{\partial^2 u}{\partial x^2} = \frac{\partial u}{\partial t}$$

- map onto a mesh with stepsize h and k

$$x_i = x_0 + ih \quad t_i = t_0 + ik$$

- Central difference approximation for spatial derivative (at fixed time)

$$\frac{\partial^2 u}{\partial x^2} = \frac{u_{j+1} - 2u_j + u_{j-1}}{h^2}$$

- Time derivative at $t = t^{n+1}$

$$\frac{du}{dt} = \frac{u^{n+1} - u^n}{k}$$

Example: Explicit finite differences

- Combining time derivative expression using spatial derivative at $t = t^n$

$$\frac{u_j^{n+1} - u_j^n}{k} = \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{h^2}$$

- Solve for u at time $n+1$ and step j

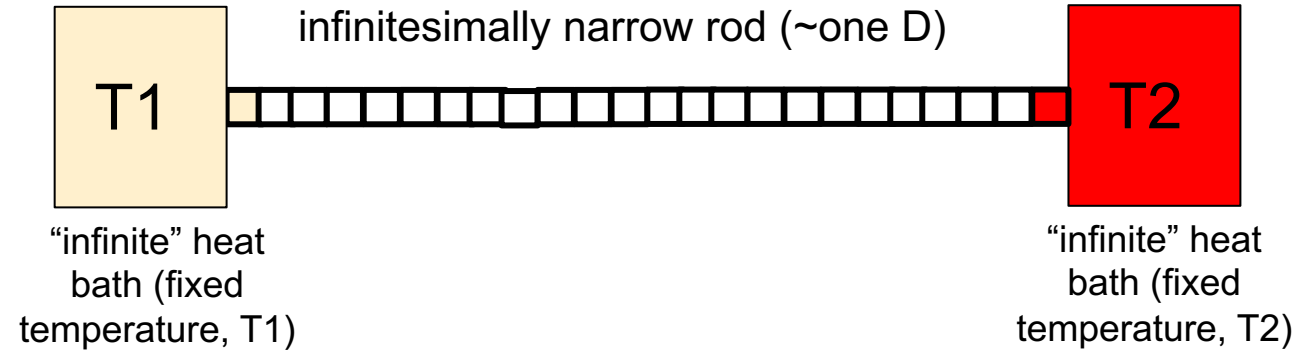
$$u_j^{n+1} = (1 - 2r)u_j^n + ru_{j-1}^n + ru_{j+1}^n \quad r = k/h^2$$

- The solution at $t = t_{n+1}$ is determined explicitly from the solution at $t = t_n$ (assume $u[t][0] = u[t][N] = \text{Constant}$ for all t).

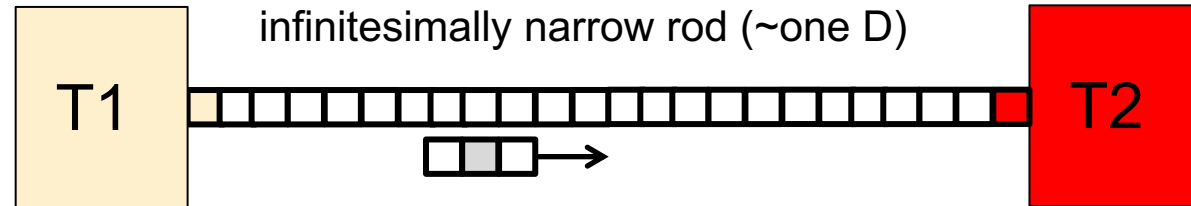
```
for (int t = 0; t < N_STEPS-1; ++t)
    for (int x = 1; x < N-1; ++x)
        u[t+1][x] = u[t][x] + r*(u[t][x+1] - 2*u[t][x] + u[t][x-1]);
```

- Explicit methods are easy to compute ... each point updated based on nearest neighbors. Converges for $r < 1/2$.

Heat Diffusion equation

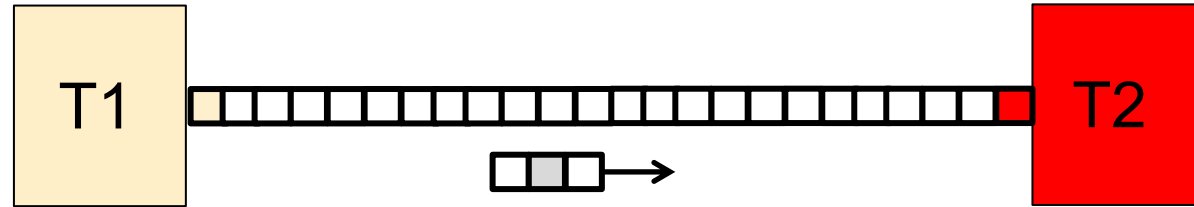


Heat Diffusion equation



Pictorially, you are sliding a three point "stencil" across the domain (u) and updating the center point at each stop.

Heat Diffusion equation



```
int main()
{
    double *u    = malloc (sizeof(double) * (N));
    double *up1  = malloc (sizeof(double) * (N));
```

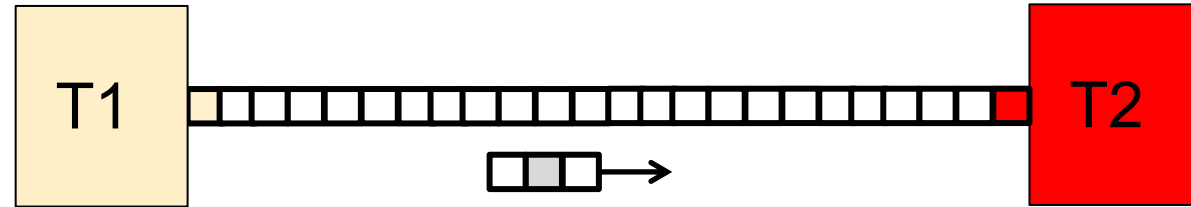
Note: I don't need the intermediate "u[t]" values hence "u" is just indexed by x.

```
    initialize_data(uk, ukp1, N, P); // init to zero, set end temperatures
    for (int t = 0; t < N_STEPS; ++t){
        for (int x = 1; x < N-1; ++x)
            up1[x] = u[x] + (k / (h*h)) * (u[x+1] - 2*u[x] + u[x-1]);
```

```
        temp = up1; up1 = u; u = temp;
    }
    return 0;
```

A well known trick with 2 arrays so I don't overwrite values from step k-1 as I fill in for step k

Heat Diffusion equation



```
int main()
{
    double *u    = malloc (sizeof(double) * (N));
    double *up1 = malloc (sizeof(double) * (N));
```

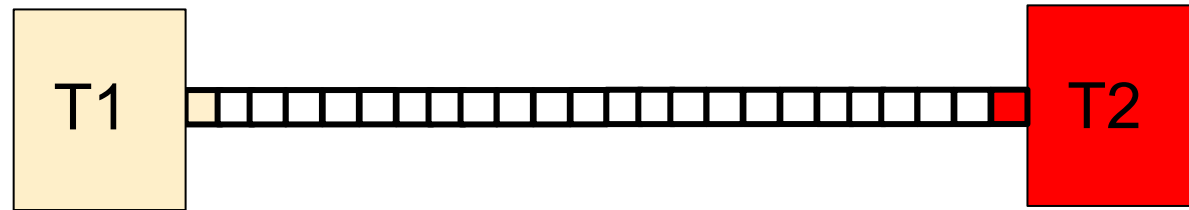
```
    initialize_data(uk, ukp1, N, P); // init to zero, set end temperatures
    for (int t = 0; t < N_STEPS; ++t){
        for (int x = 1; x < N-1; ++x)
            up1[x] = u[x] + (k / (h*h)) * (u[x+1] - 2*u[x] + u[x-1]);
```

```
        temp = up1; up1 = u; u = temp;
    }
    return 0;
```

How would
you parallelize
this program?

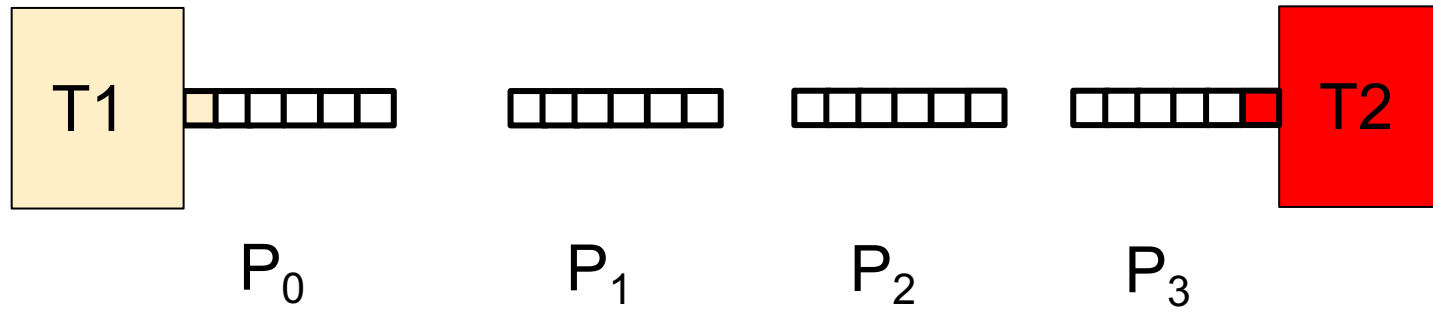
Heat Diffusion equation

- Start with our original picture of the problem ... a one dimensional domain with end points set at a fixed temperature.



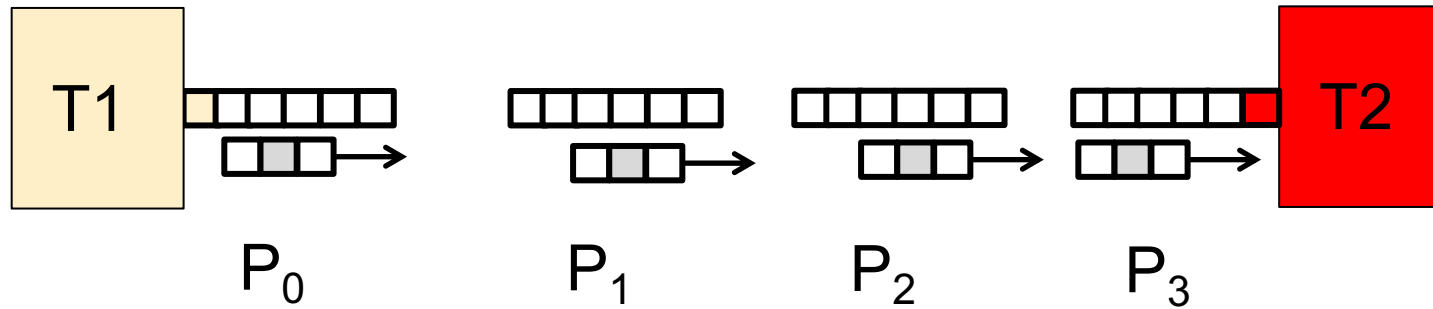
Heat Diffusion equation

- Break it into chunks assigning one chunk to each process.



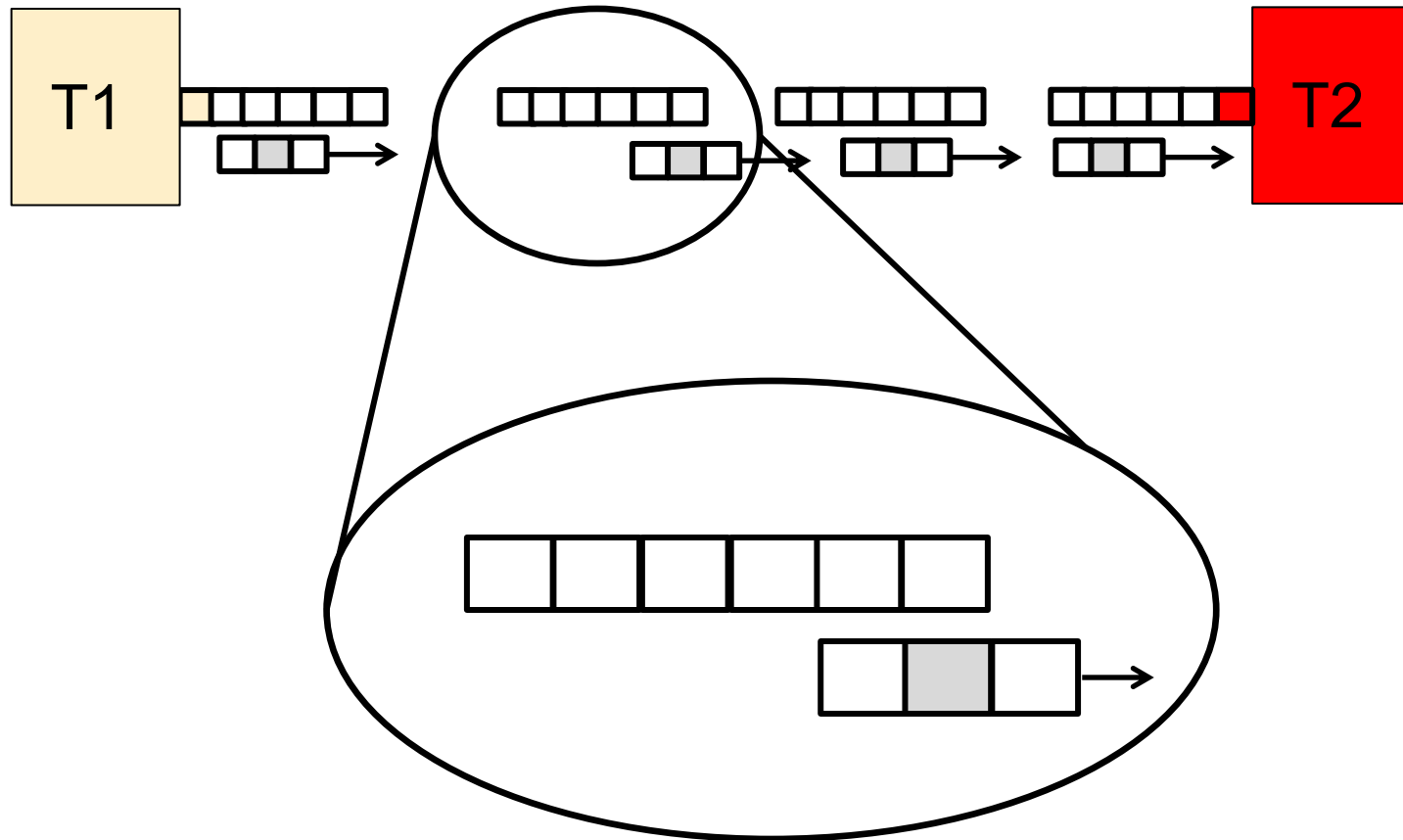
Heat Diffusion equation

- Each process works on its own chunk ... sliding the stencil across the domain to update its own data.



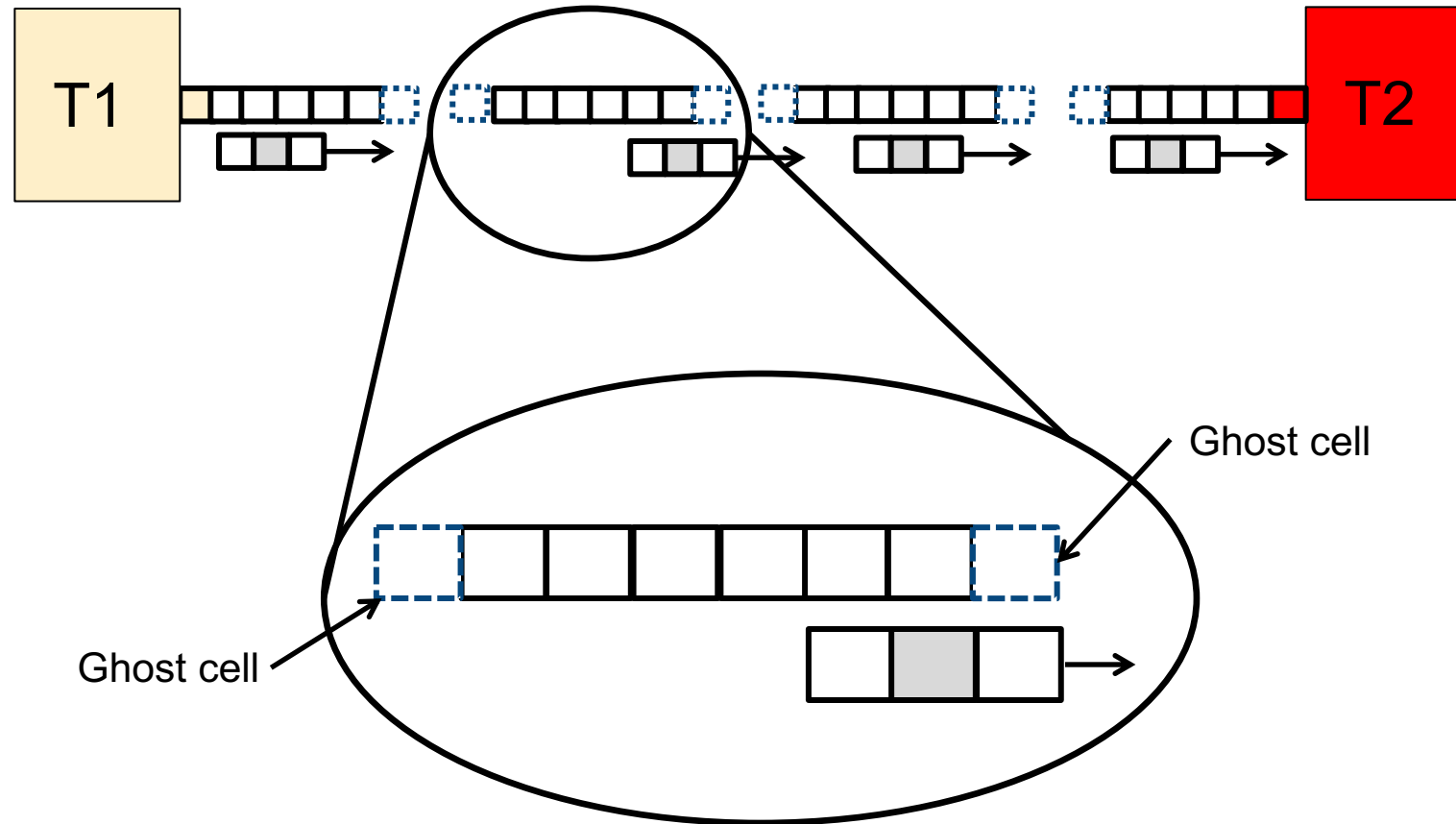
Heat Diffusion equation

- What about the ends of each chunk ... where the stencil will run off the end and hence have missing values for the computation?



Heat Diffusion equation

- We add ghost cells to the ends of each chunk, update them with the required values from neighbor chunks at each time step ... hence giving the stencil everything it needs on any given chunk to update all of its values.

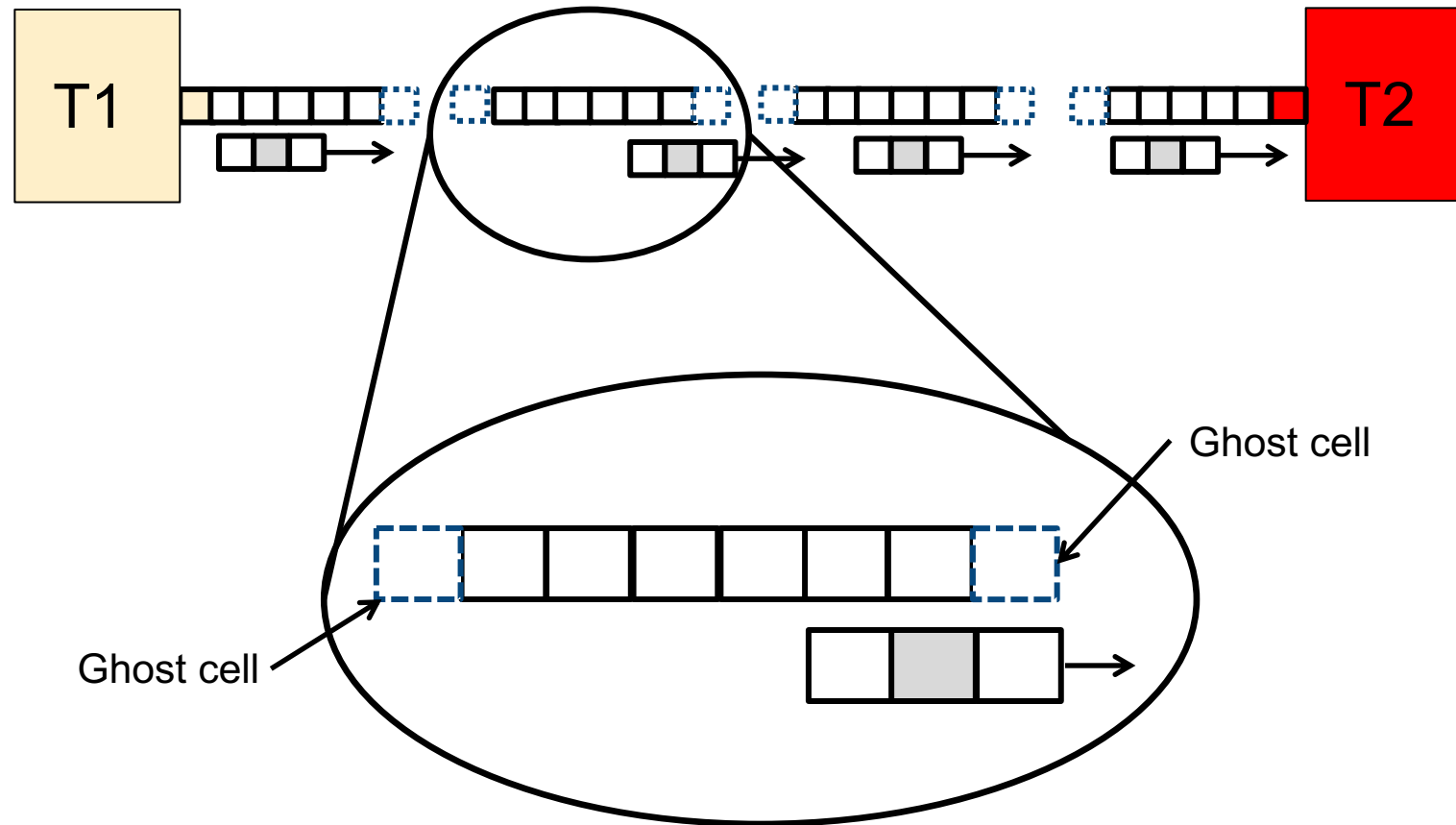


Design Pattern: Geometric Decomposition

- Use when:
 - The problem is organized around a central data structure that can be decomposed into smaller segments (chunks) that can be updated concurrently.
- Solution
 - Typically, the data structure is updated iteratively where a new value for one chunk depends on neighboring chunks.
 - The computation breaks down into three components: (1) exchange boundary data, (2) update the interiors of each chunk, and (3) update boundary regions. The optimal size of the chunks is dictated by the properties of the memory hierarchy.
- Note:
 - This pattern is often used with the Structured Mesh and linear algebra computational strategy pattern.

The Geometric Decomposition Pattern

- This is an instance of a very important design pattern ... the Geometric decomposition pattern.



Heat Diffusion MPI Example

```
MPI_Init (&argc, &argv);
MPI_Comm_size (MPI_COMM_WORLD, &P);
MPI_Comm_rank (MPI_COMM_WORLD, &myID);
double *u      = malloc (sizeof(double) * (2 + N/P)) // include "Ghost Cells"
double *up1 = malloc (sizeof(double) * (2 + N/P)); // to hold values
                                                    // from my neighbors

initialize_data(uk, ukp1, N, P);
for (int t = 0; t < N_STEPS; ++t){
    if (myID != 0) MPI_Send (&u[1], 1, MPI_DOUBLE, myID-1, 0, MPI_COMM_WORLD);
    if (myID != P-1) MPI_Recv (&u[N/P+1], 1, MPI_DOUBLE, myID+1, 0, MPI_COMM_WORLD, &status);
    if (myID != P-1) MPI_Send (&u[N/P], 1, MPI_DOUBLE, myID+1, 0, MPI_COMM_WORLD);
    if (myID != 0) MPI_Recv (&u[0], 1, MPI_DOUBLE, myID-1, 0, MPI_COMM_WORLD, &status);
```

```
    for (int x = 2; x <= N/P; ++x)
        up1[x] = u[x] + (k / (h*h)) * (u[x+1] - 2*u[x] + u[x-1]);
    if (myID != 0)
        up1[1] = u[1] + (k / (h*h)) * (u[1+1] - 2*u[1] + u[1-1]);
    if (myID != P-1)
        up1[N/P] = u[N/P] + (k/(h*h)) * (u[N/P+1] - 2*u[N/P] + u[N/P-1]);
    temp = up1; up1 = u; u = temp;

} // End of for (int t ...) loop

MPI_Finalize();
return 0;
```

We write/explain
this part first and
then address the
communication and
data structures

Heat Diffusion MPI Example

```
/* continued from previous slide */
```

Temperature fields using local data and values from ghost cells.

```
for (int x = 2; x <= N/P; ++x)
```

```
    up1[x] = u[x] + (k / (h*h)) * (u[x+1] - 2*u[x] + u[x-1]);
```

```
if (myID != 0)
```

```
    up1[1] = u[1] + (k / (h*h)) * (u[1+1] - 2*u[1] + u[1-1]);
```

$u[0]$ and $u[N/P+1]$
are the ghost
cells

```
if (myID != P-1)
```

```
    up1[N/P] = u[N/P] + (k/(h*h)) * (u[N/P+1] - 2*u[N/P] + u[N/P-1]);
```

```
temp = up1; up1 = u; u = temp;
```

```
} // End of for (int t ...) loop
```

```
MPI_Finalize();
```

```
return 0;
```

Note I was lazy and assume N was evenly divided by P . Clearly, I'd never do this in a "real" program.

Heat Diffusion MPI Example

```
MPI_Init (&argc, &argv);
MPI_Comm_size (MPI_COMM_WORLD, &P);
MPI_Comm_rank (MPI_COMM_WORLD, &myID);
double *u      = malloc (sizeof(double) * (2 + N/P)) // include "Ghost Cells"
double *up1 = malloc (sizeof(double) * (2 + N/P)); // to hold values
                                                    // from my neighbors

initialize_data(uk, ukp1, N, P);
for (int t = 0; t < N_STEPS; ++t){
    if (myID != 0)
        MPI_Send (&u[1], 1, MPI_DOUBLE, myID-1, 0, MPI_COMM_WORLD);

    if (myID != P-1)
        MPI_Recv (&u[N/P+1], 1, MPI_DOUBLE, myID+1, 0, MPI_COMM_WORLD, &status);

    if (myID != P-1)
        MPI_Send (&u[N/P], 1, MPI_DOUBLE, myID+1, 0, MPI_COMM_WORLD);

    if (myID != 0)
        MPI_Recv (&u[0], 1, MPI_DOUBLE, myID-1, 0, MPI_COMM_WORLD, &status);
/* continued on next slide */
```

1D PDE solver ... the simplest "real" message passing code I can think of. Note: edges of domain held at a fixed temperature

Send my "right" boundary value to my "right" neighbor

Receive my "left" ghost cell from my "left" neighbor

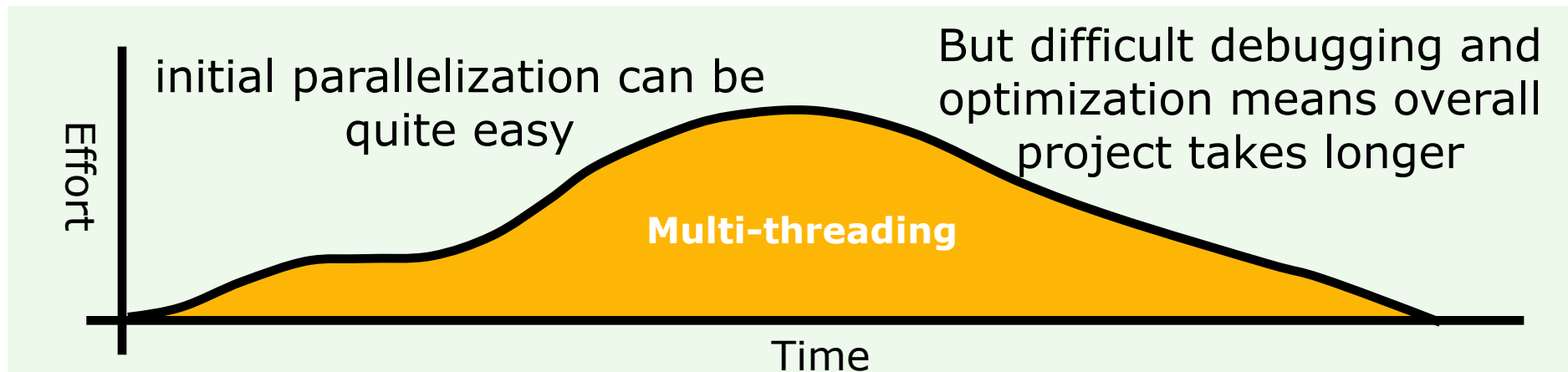
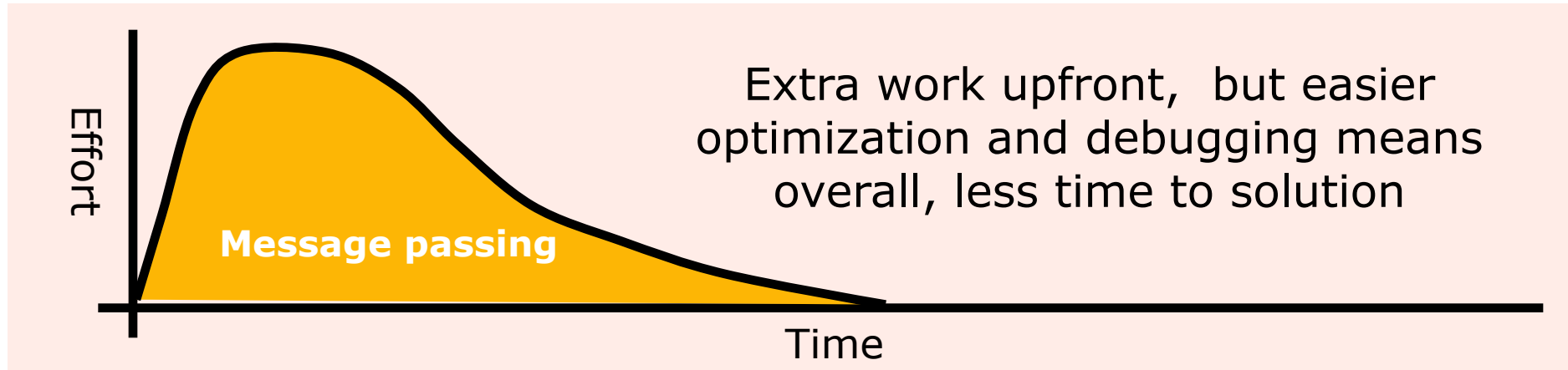
Send my "left" boundary value to my "left" neighbor

Receive my "right" ghost cell from my "right" neighbor

MPI is huge!!!

- MPI has over 430 functions!!!
 - Many forms of message passing
 - Full range of collectives (such as reduction)
 - dynamic process management
 - Shared memory
 - and much more
- Most programs, however use around a dozen different constructs ... so it's not as hard to learn as it may seem.

Does a shared address space make programming easier?



Proving that a shared address space program using semaphores is race free is an NP-complete problem*

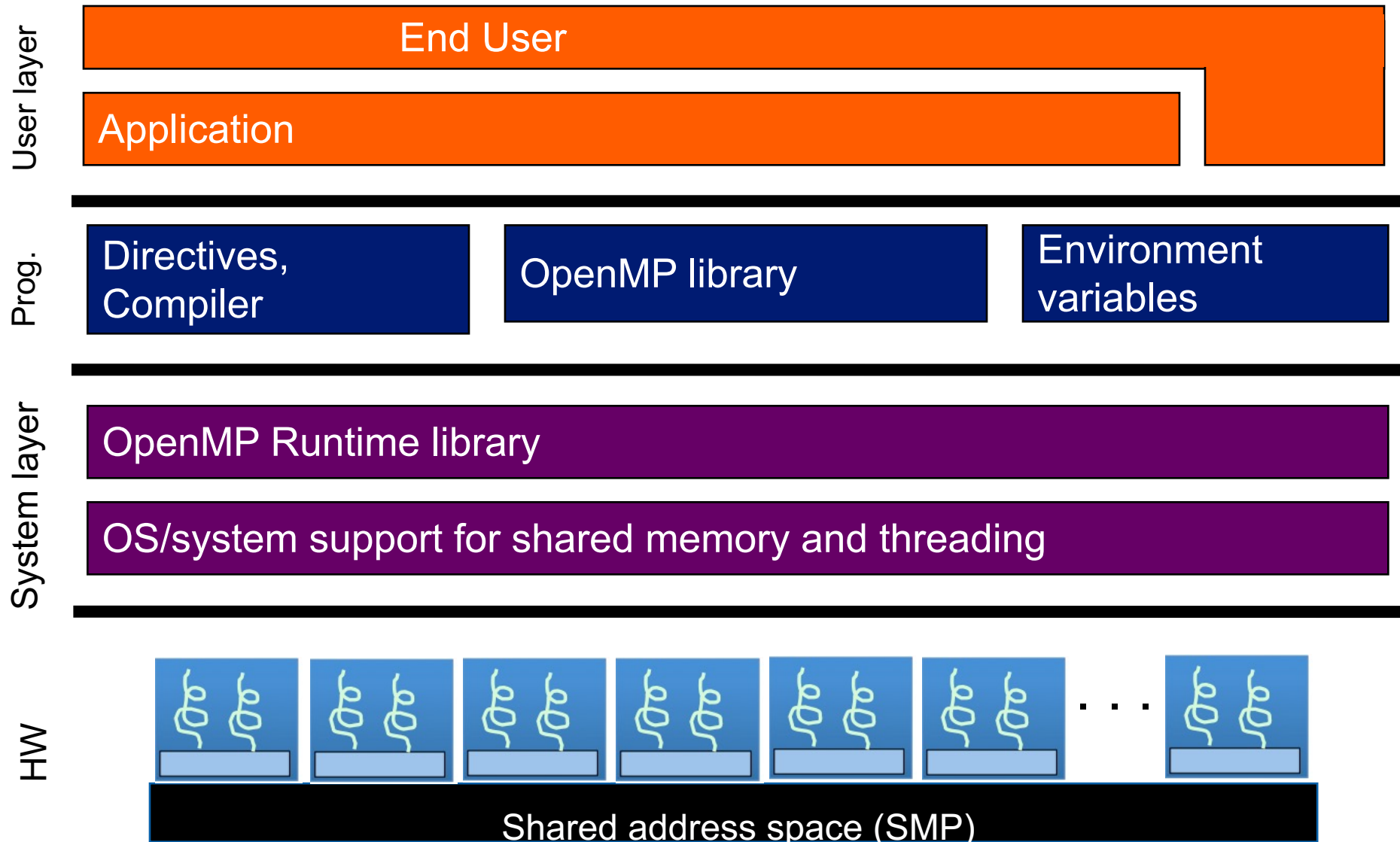
The Big Three

- 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)
- 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.

The “new”
kid on the
block ...
GPUs

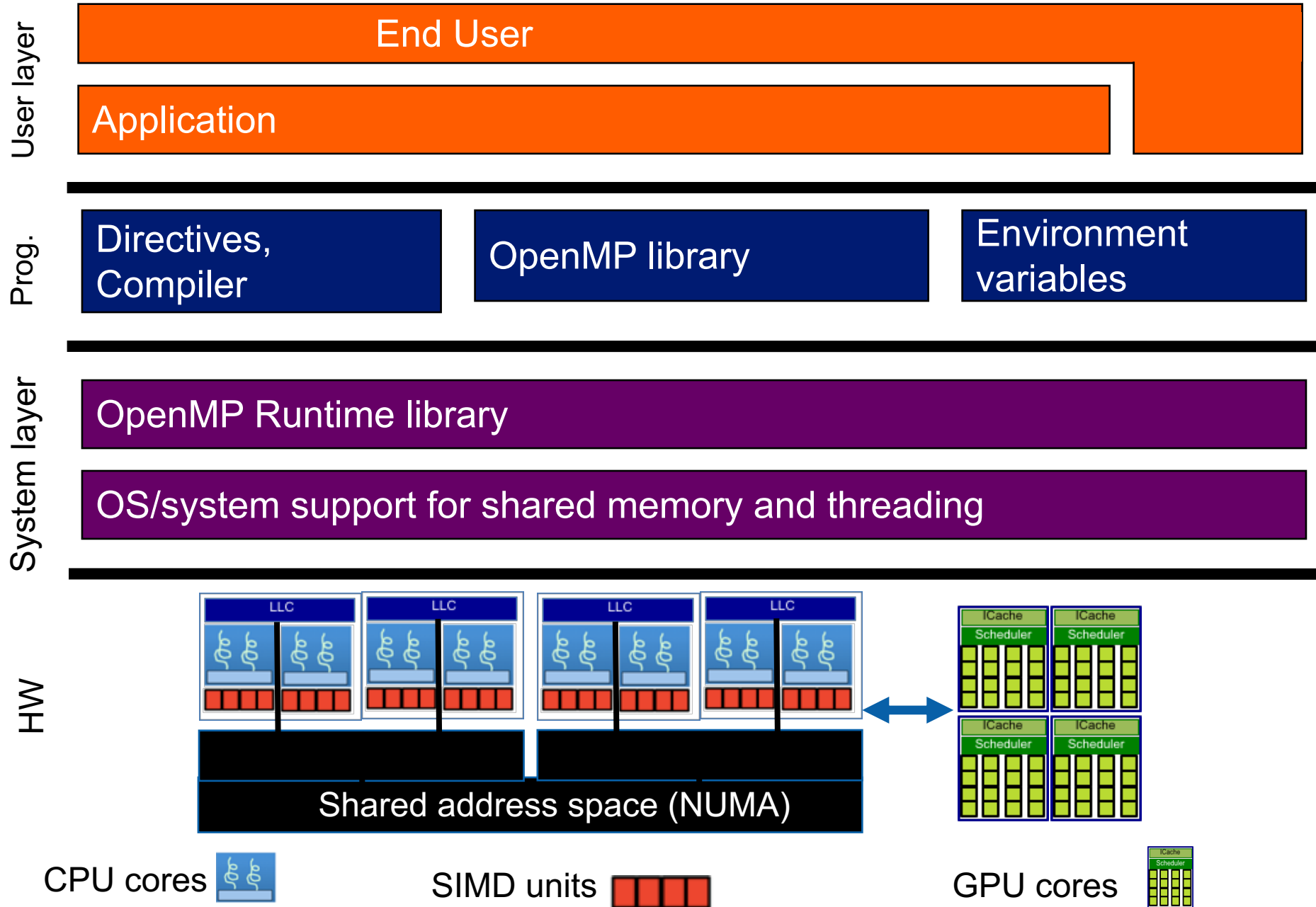


OpenMP Basic Definitions: Basic Solution Stack

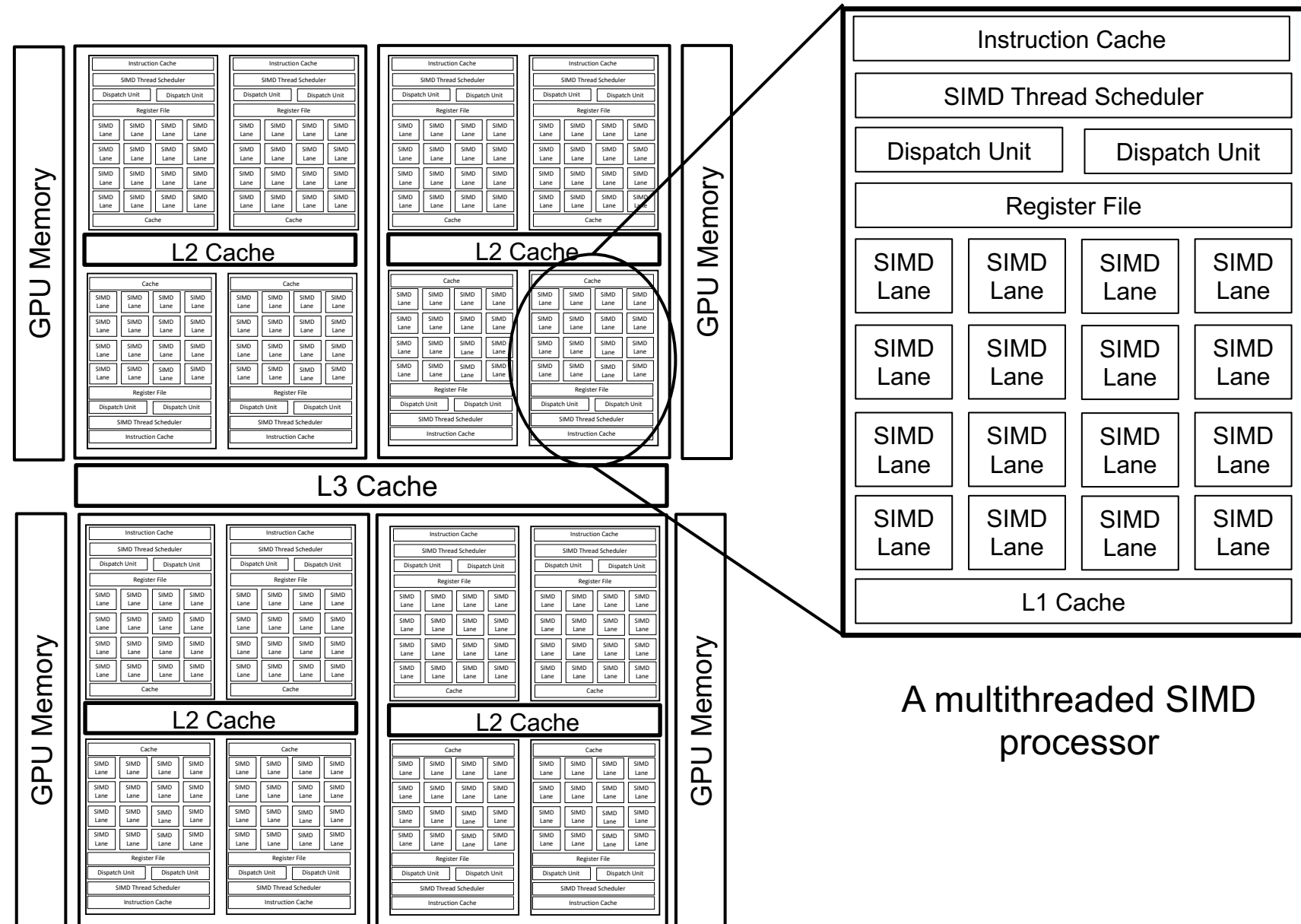


For the OpenMP Common Core, we focus on Symmetric Multiprocessor Case
i.e., lots of threads with “equal cost access” to memory

OpenMP Basic Definitions: Solution stack

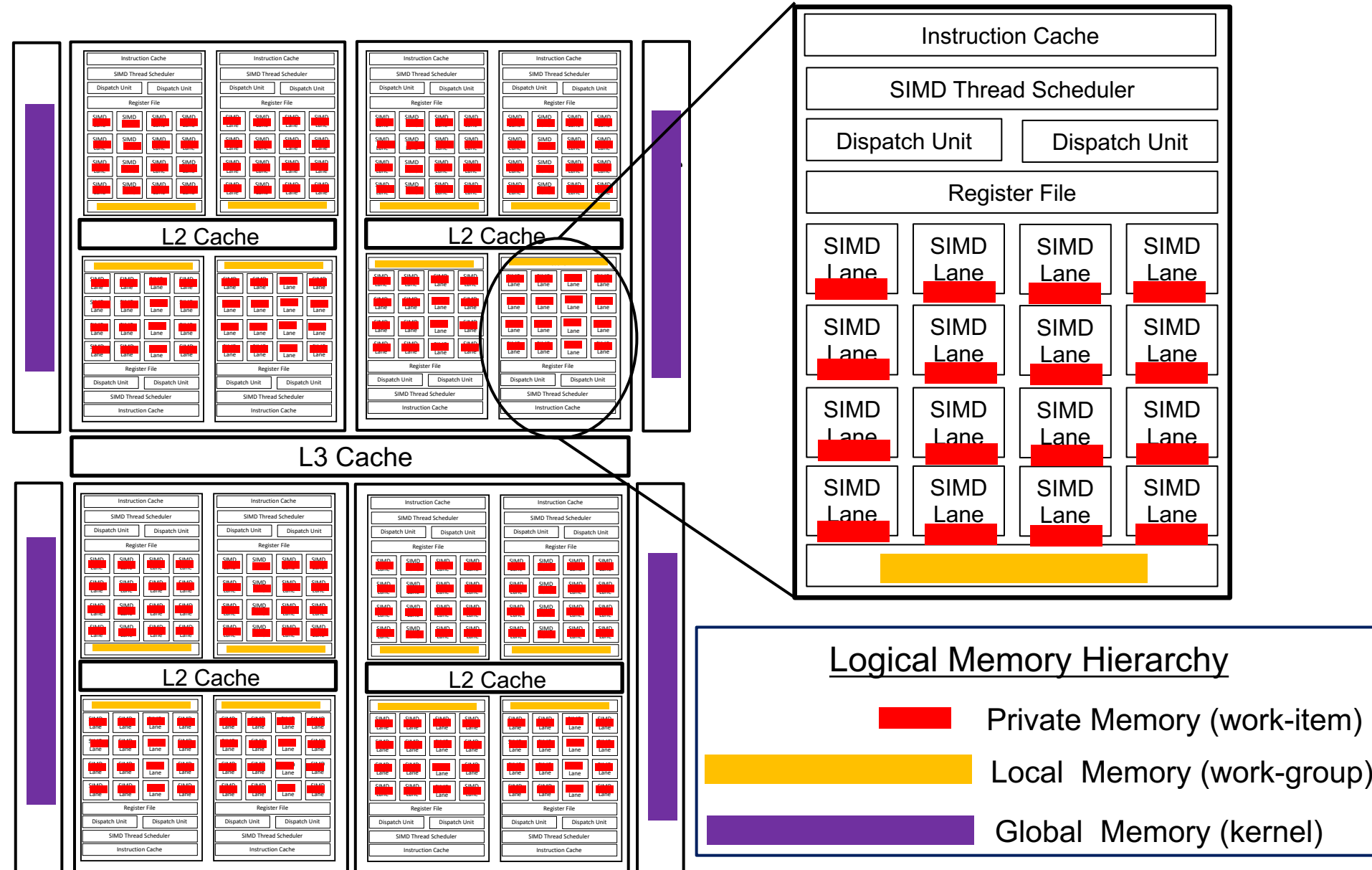


A Generic GPU (following Hennessey and Patterson)



A multithreaded SIMD processor

A Generic GPU (following Hennessey and Patterson)



The “BIG idea” of GPU programming

Traditional loops

```
void
trad_mul(int n,
         const float *a,
         const float *b,
         float *c)
{
    int i;
    for (i=0; i<n; i++)
        c[i] = a[i] * b[i];
}
```



Data Parallel OpenCL

```
kernel void
dp_mul(global const float *a,
        global const float *b,
        global float *c)
{
    int id = get_global_id(0);

    c[id] = a[id] * b[id];
} // execute over "n" work-items
```

This is just the kernel code. The host code running on the CPU is much more complicated.

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

1. Turn source code into a scalar work-item

```
extern void reduce( __local float*, __global float*);

__kernel void pi( const int niters, float step_size,
                 __local float* l_sums, __global float* p_sums)
{
    int n_wrk_items = get_local_size(0);
    int loc_id      = get_local_id(0);
    int grp_id      = get_group_id(0);
    float x, accum = 0.0f;  int i, istart, iend;

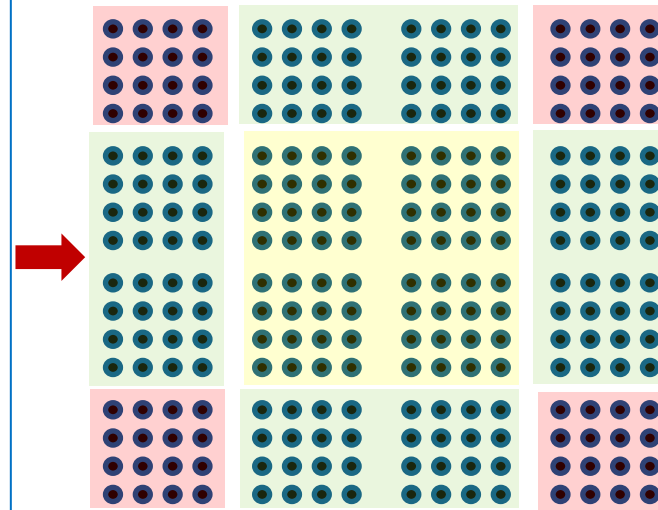
    istart = (grp_id * n_wrk_items + loc_id) * niters;
    iend   = istart + niters;

    for(i= istart; i<iend; i++){
        x = (i+0.5f)*step_size;  accum += 4.0f/(1.0f+x*x); }

    l_sums[loc_id] = accum;
    barrier(CLK_LOCAL_MEM_FENCE);
    reduce(l_sums, p_sums);
}
```

This is OpenCL kernel 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

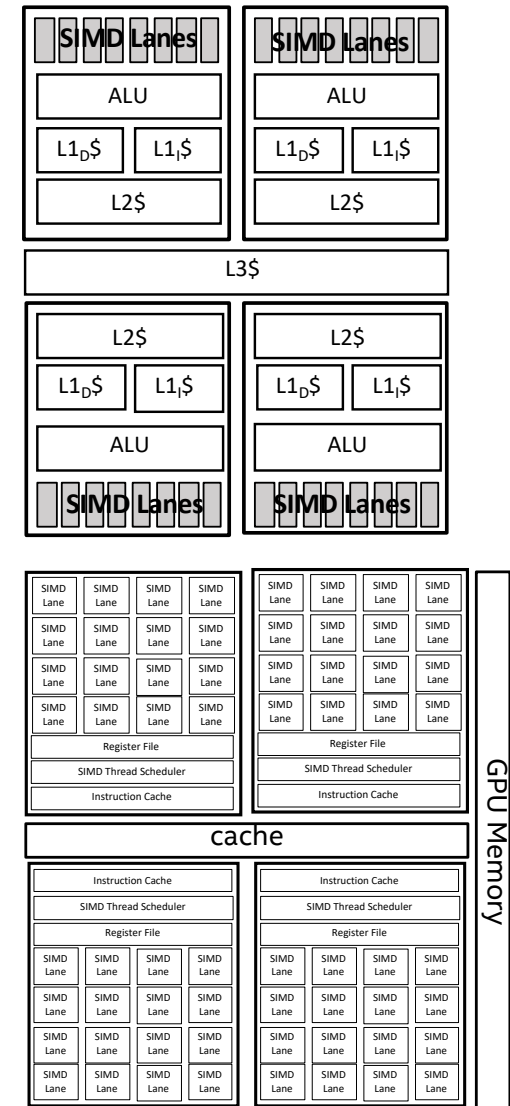
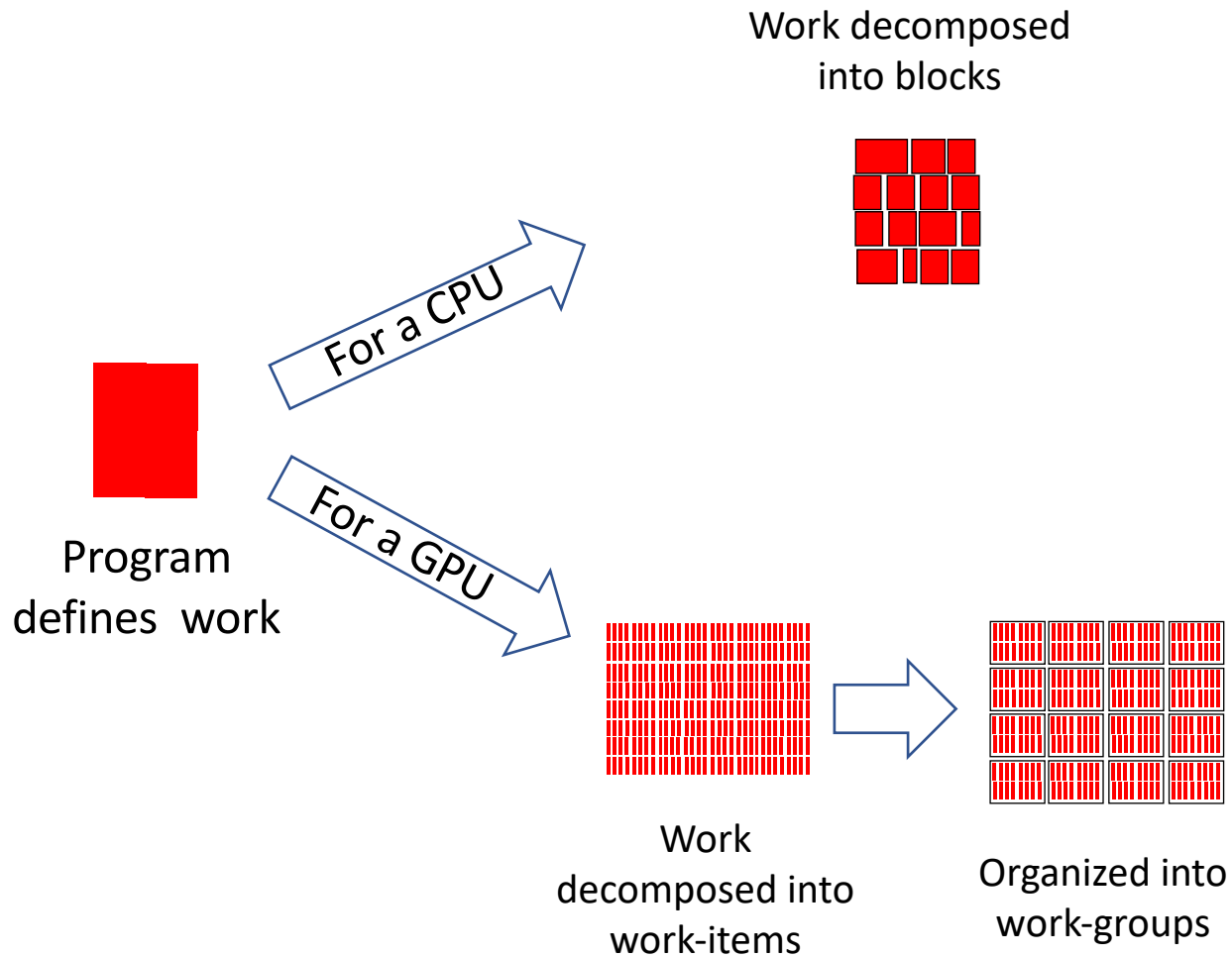
4. Run on hardware designed around the same SIMT execution model



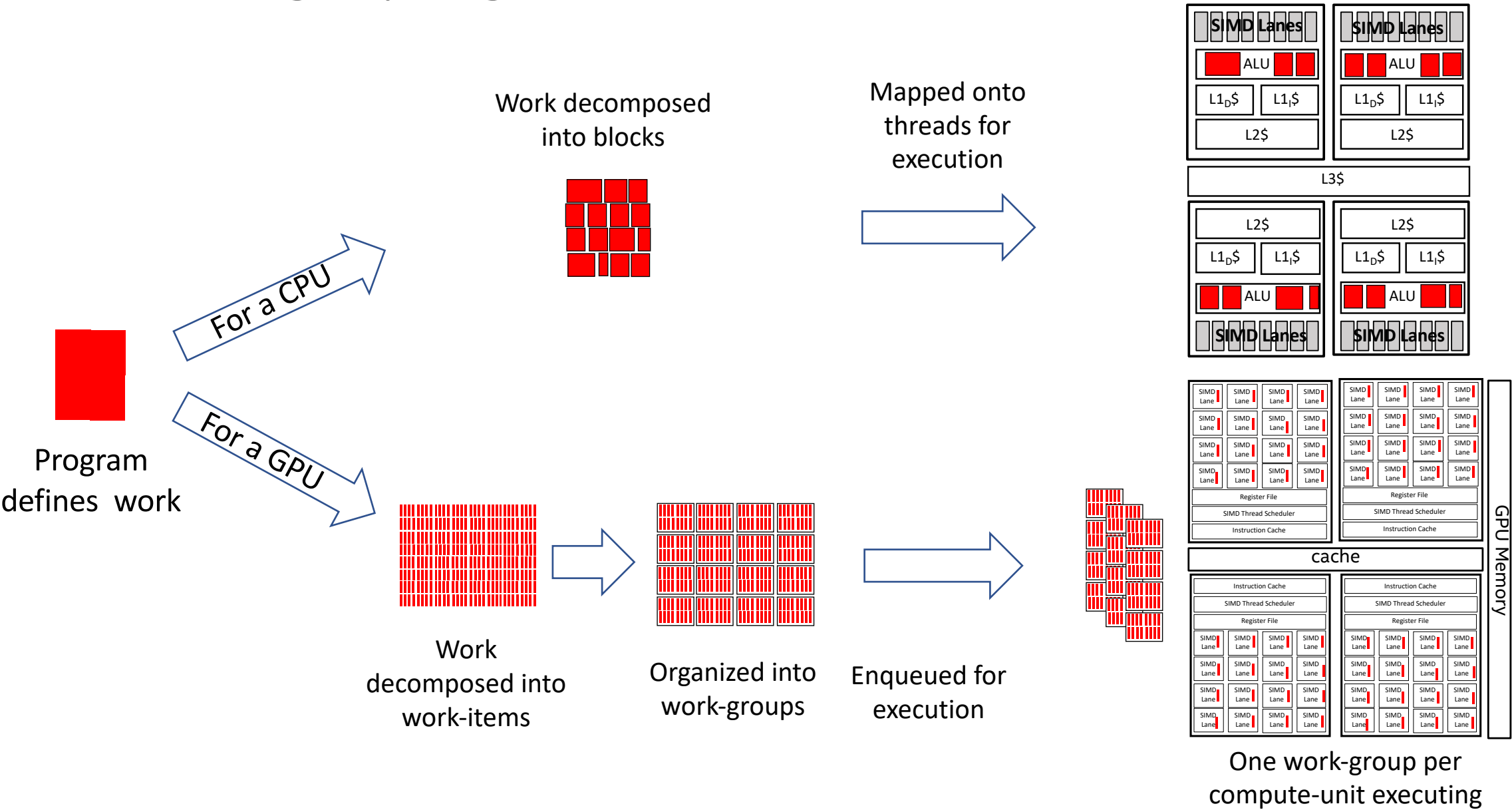
GPU terminology is Broken (sorry about that)

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

Executing a program on CPUs and GPUs

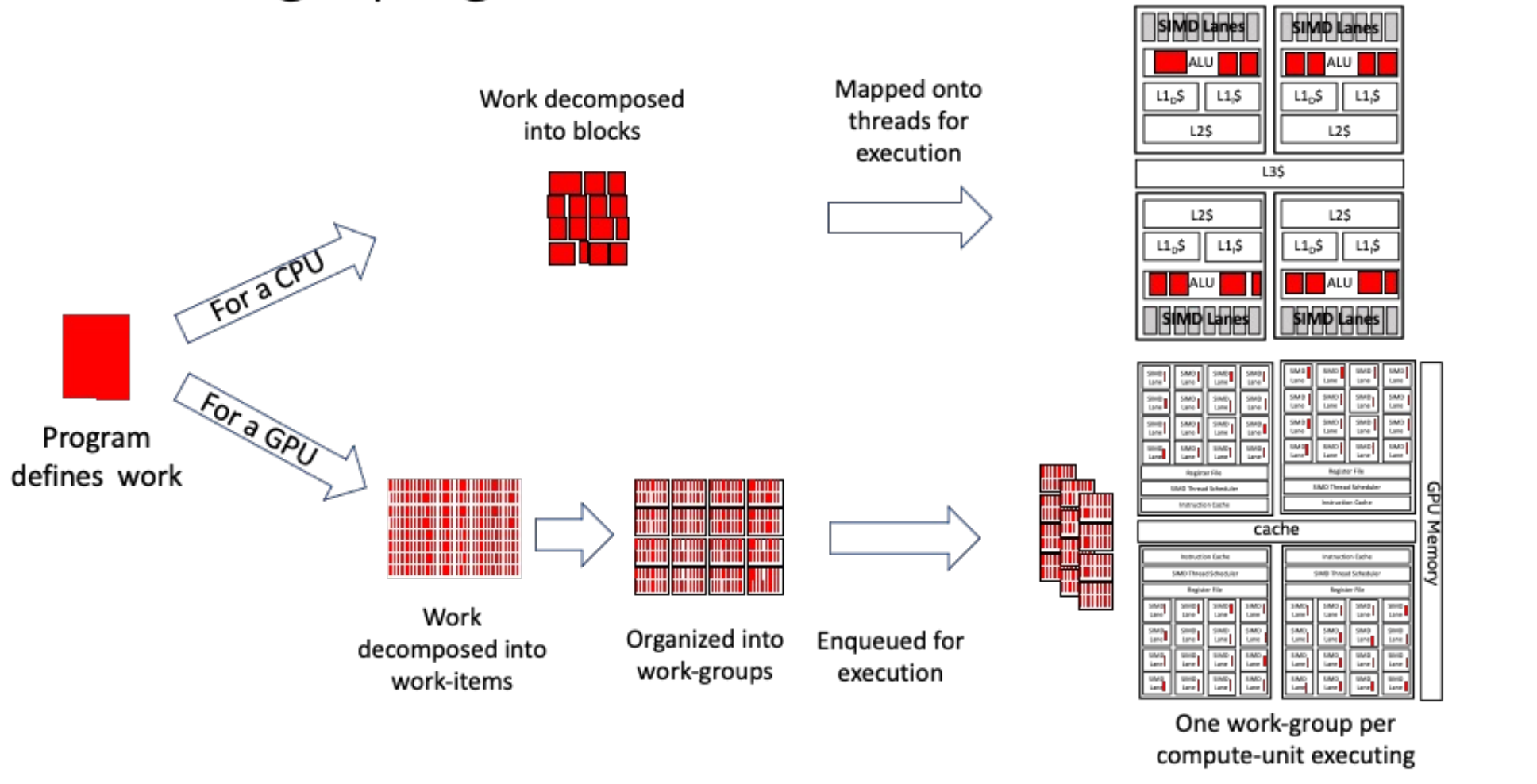


Executing a program on CPUs and GPUs



CPU/GPU execution modes

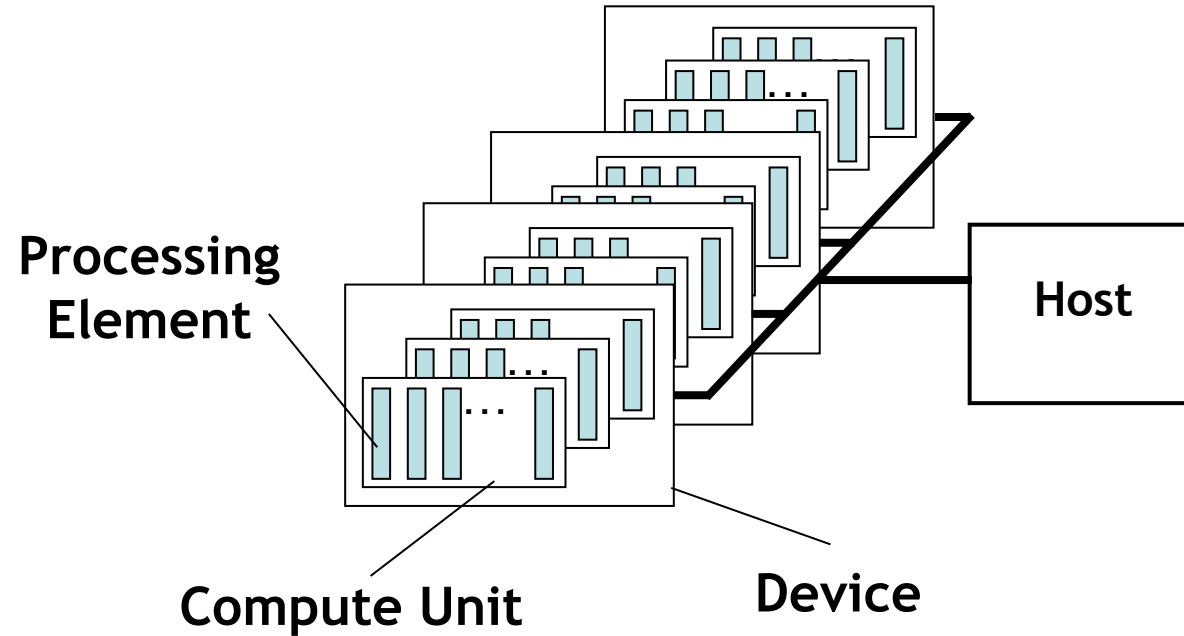
Executing a program on CPUs and GPUs



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.

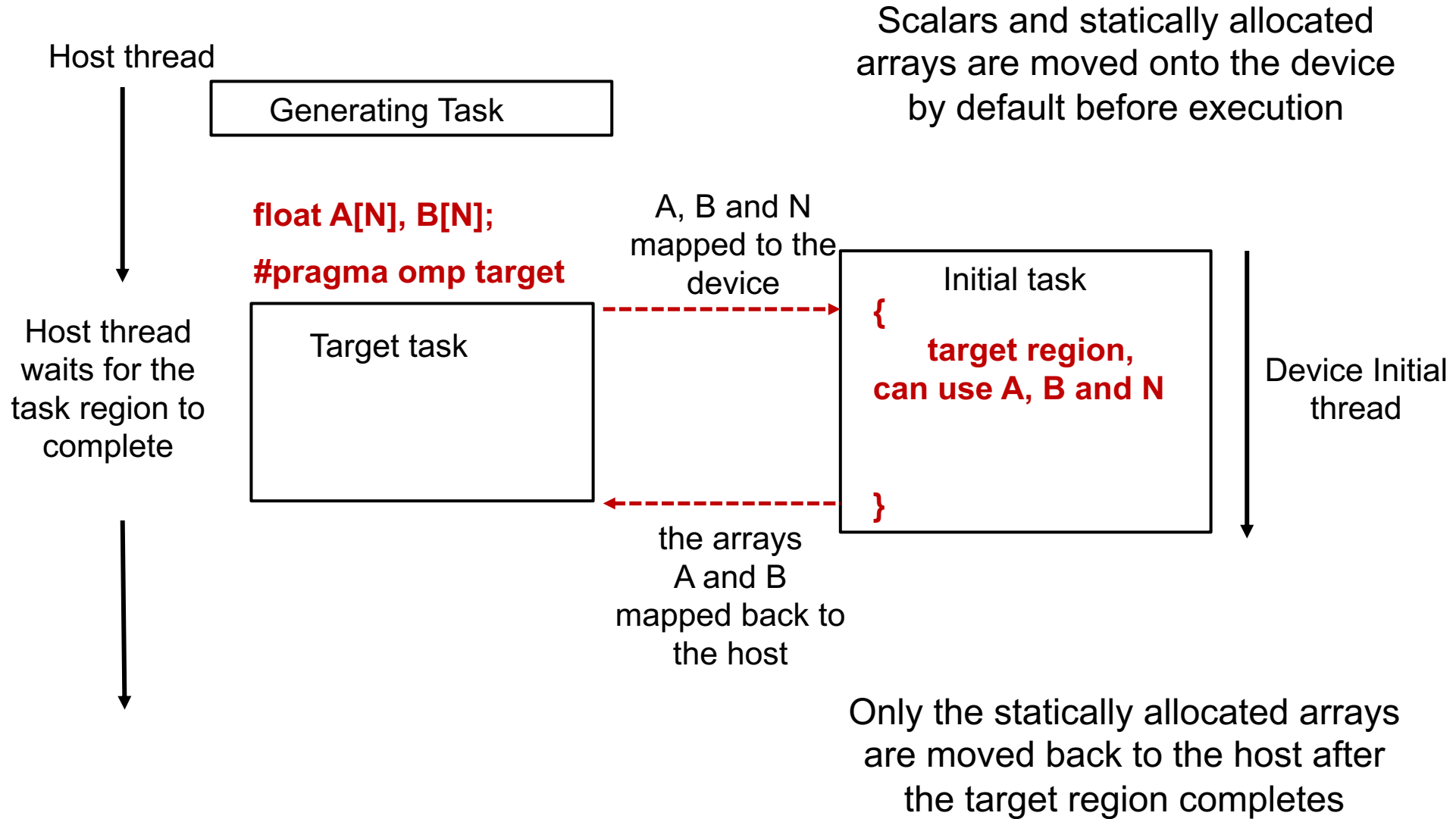
A Generic Host/Device Platform Model



- 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



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.

So lets 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

What about pointers?

implicit movement with a target region

- Pointers and their data:
 - *Example: arrays allocated on the heap*
 - `double *A = malloc(sizeof(double)*1000);`
 - The pointer value will be mapped.
 - But the data it points to **will not** be mapped by default.

Explicit Data Sharing

- We *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 = 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!  
    }  
}
```

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 (device to host copy). On entering the region, initial value of the variable 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)**.
- For pointers you must use array section notation ..
 - **map(to:a[0:N])**. Notation is **A[lower-bound : length]**

Moving arrays 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.

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
$$X_{\text{new}} = (b - (L+U)x_{\text{old}})/D$$
- 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 (Par Targ, 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 (Par Targ, 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
NVIDIA® 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;
```

Typically over 4000 iterations!

```
#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];
```

```
}
```

For each iteration, **copy to** device
(3*Ndim+Ndim²)*sizeof(TYPE) bytes

```
// 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;
```

```
}
```

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

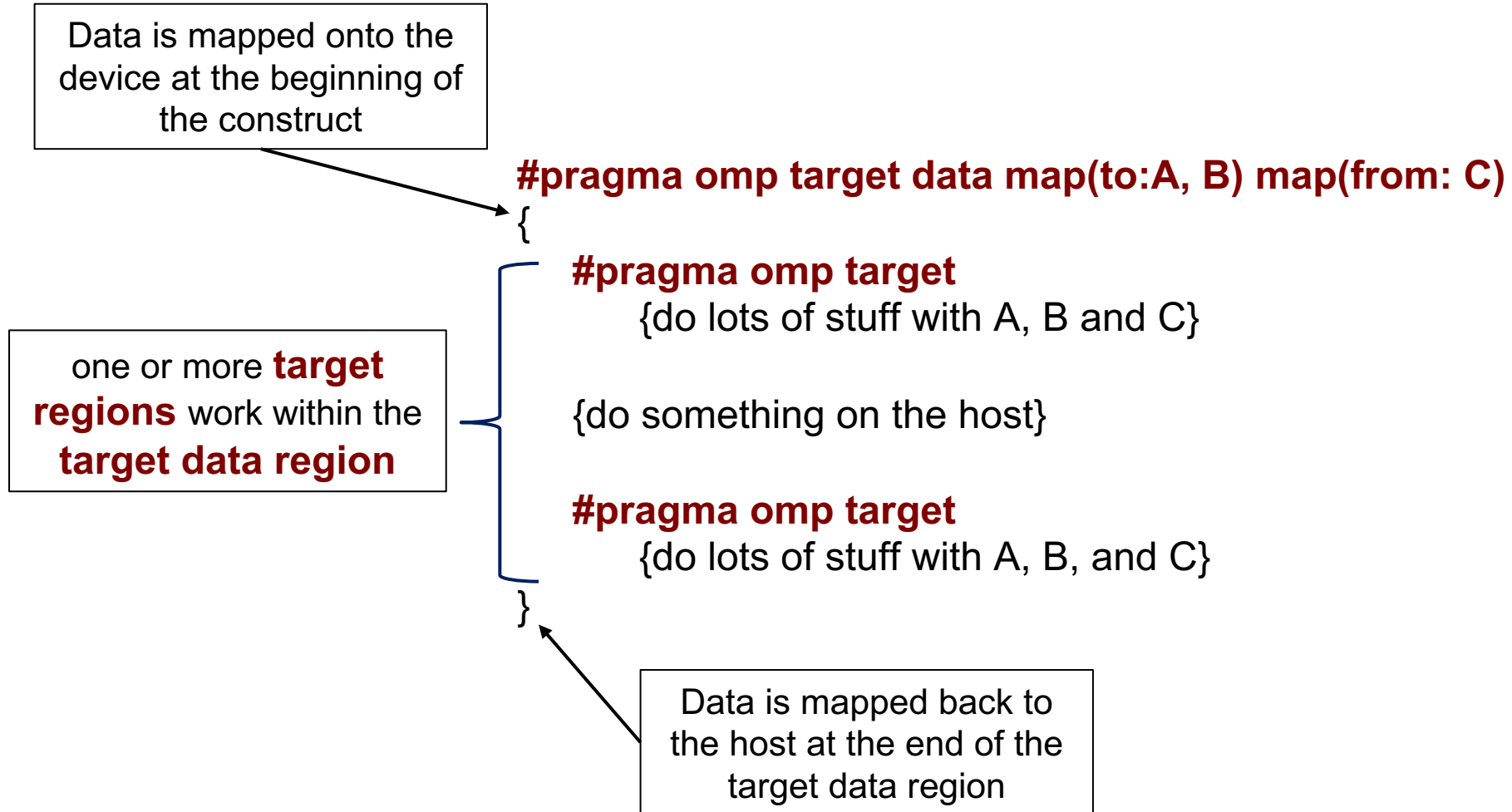
For each iteration, **copy to**
device
2*Ndim*sizeof(TYPE) bytes

```
conv = sqrt((double)conv);
```

```
}
```

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: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) 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;
```

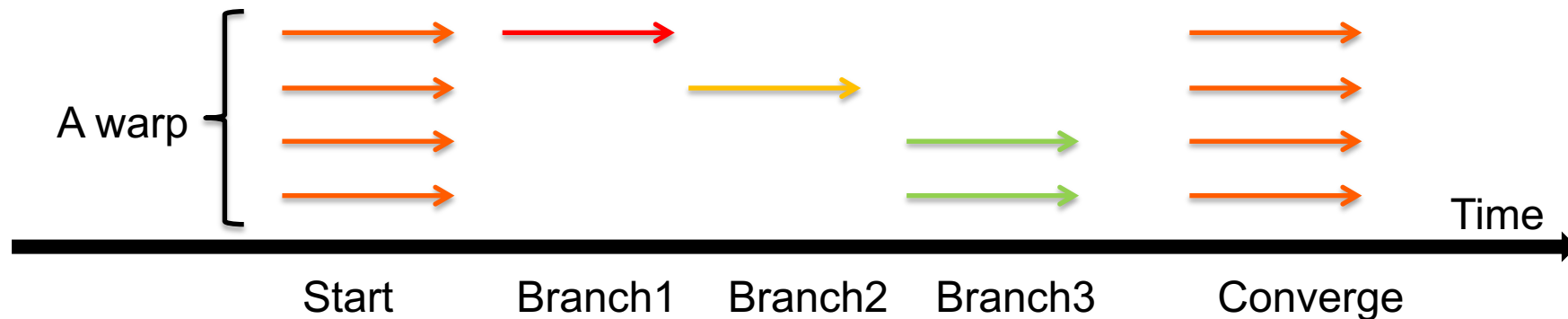
```
    xnew = tmp;
```

```
} // end while loop
```

System	Implementation	Ndim = 4096
NVIDIA® 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

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

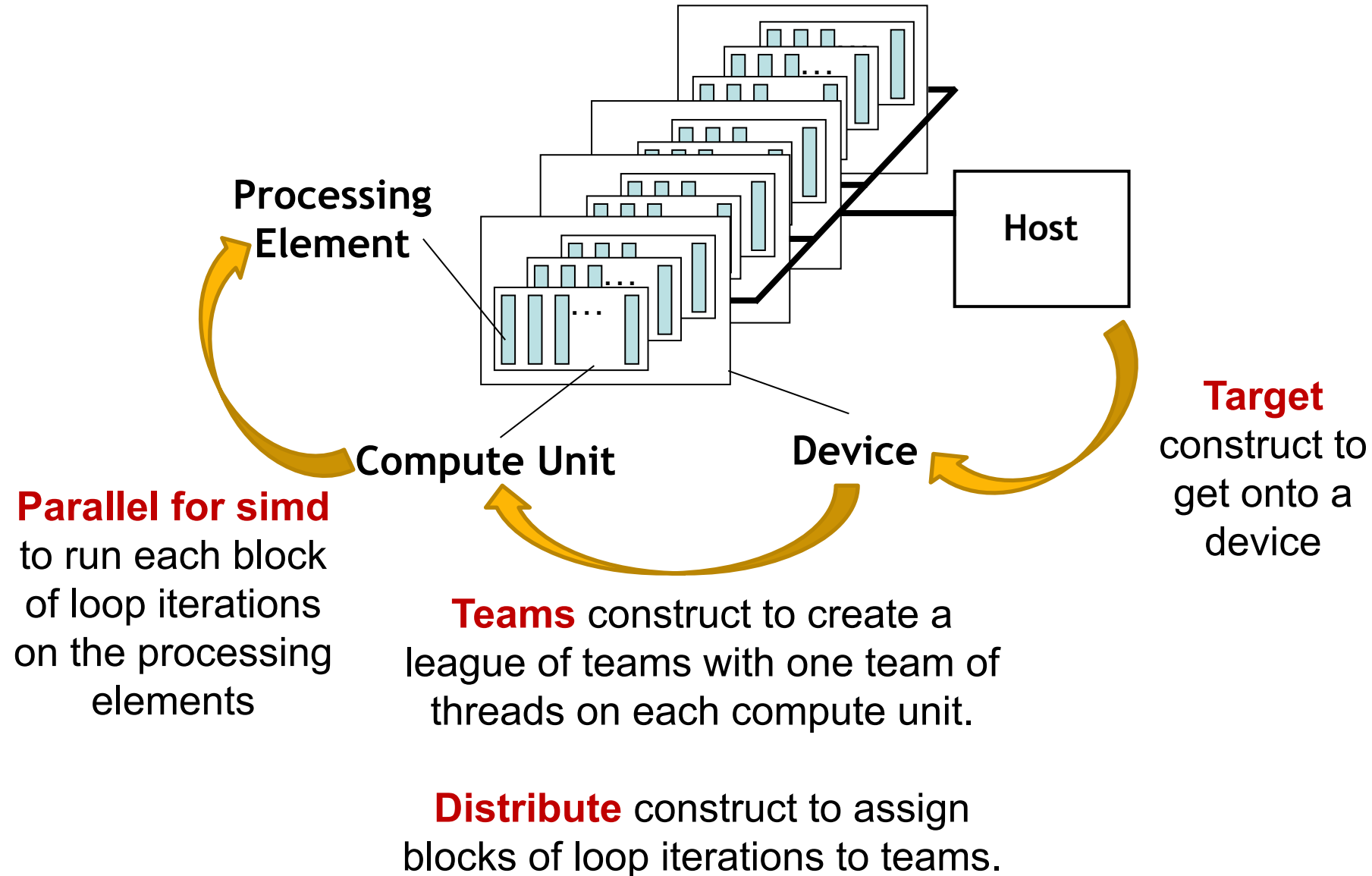
Jacobi Solver (Target Data/branchless/coalesced mem, 2/2)

```
//
// 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
NVIDIA® 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

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

Our host/device Platform Model and OpenMP



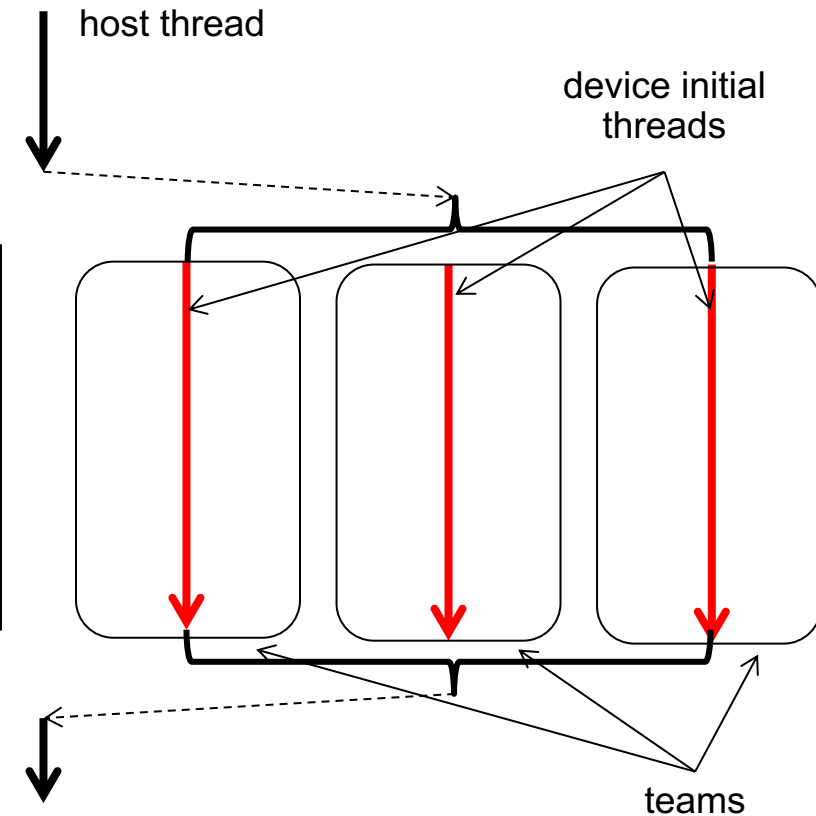
teams and distribute constructs

- 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++)  
...
```

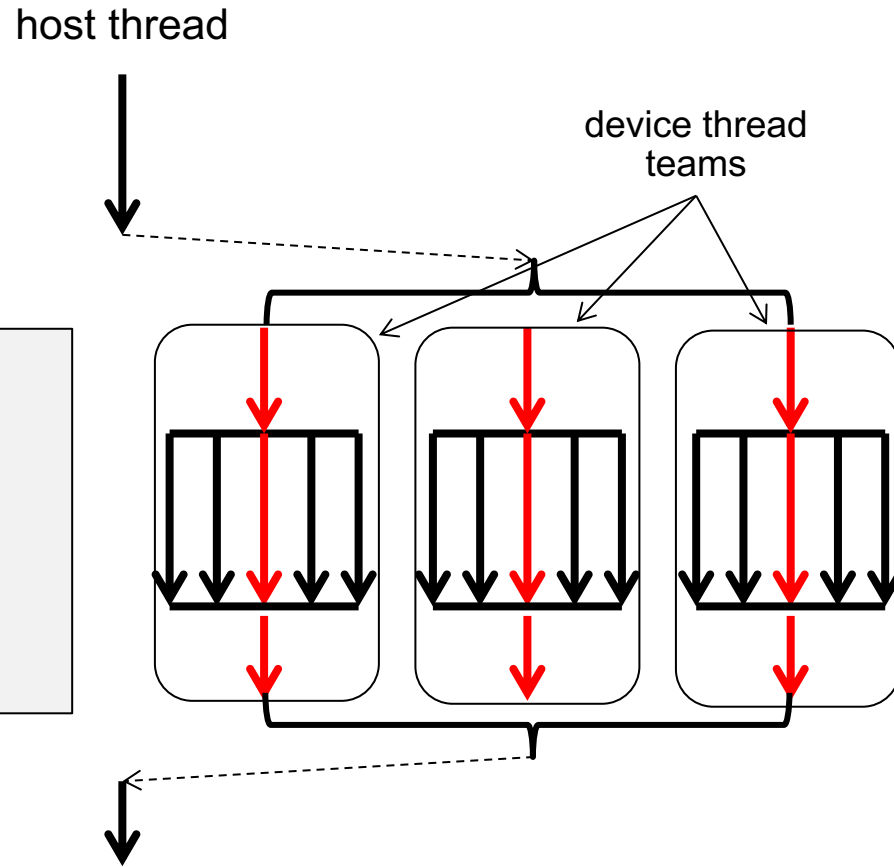


- Transfer execution control to **MULTIPLE** device initial threads
- Workshare loop iterations across the initial threads.

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++)  
...
```



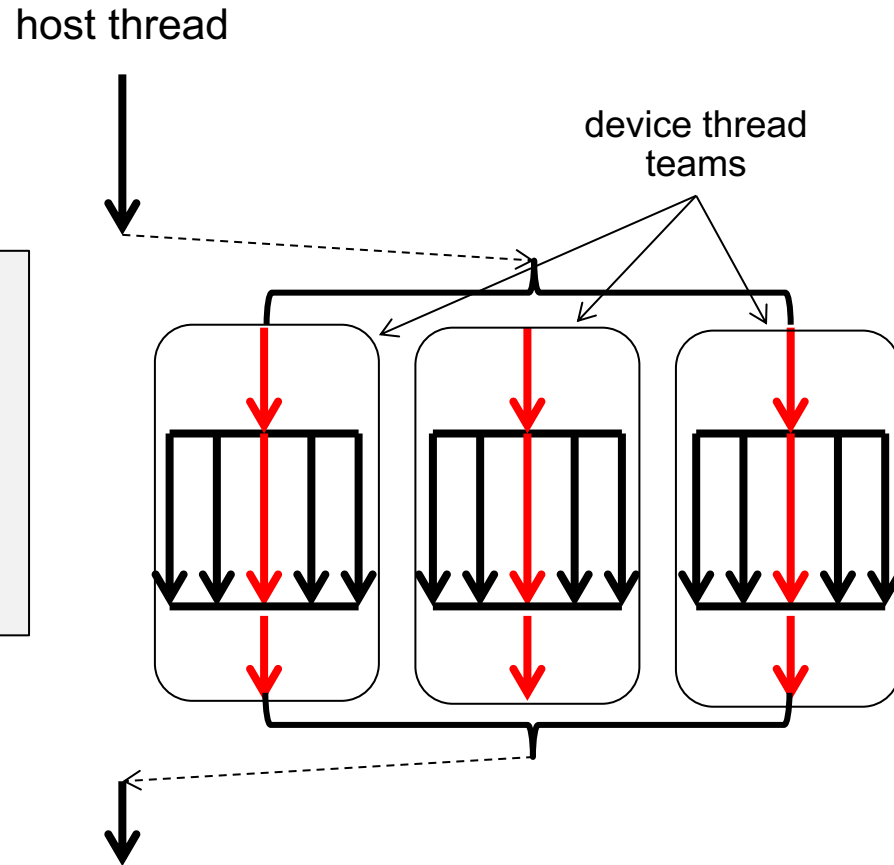
- Transfer execution control to **MULTIPLE** device initial threads
 - Workshare loop iterations across the initial threads (teams distribute)
- Each initial thread becomes the primary* thread in a thread team
 - Workshare loop iterations across the threads in a team (parallel for)

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

- 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++)  
...
```



- 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)

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 SIMT 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.
 - **OpenMP**: Mixes multithreading and SIMT. Semantics are prescriptive which makes it more verbose. A truly Open standard supported by all the key GPU players.
 - Downside: Poor compiler support so far ... but that will change over the next couple years.

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 $C = A + B$

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

```
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.

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

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

```
#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 ++;
}
```

Copy A back out to host
... but only once

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

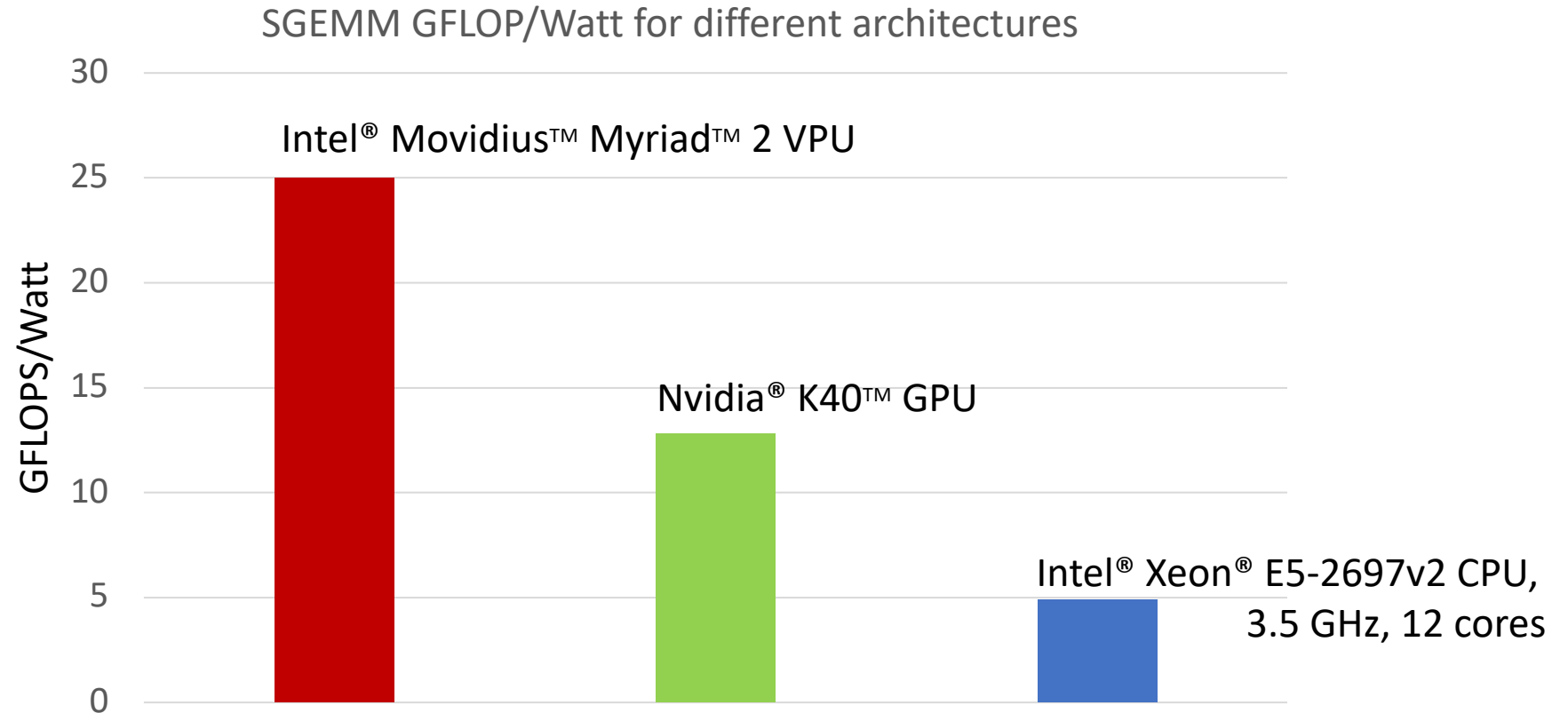
Why so many ways to do the same thing?

- 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.

What does the future hold for parallel programming?

If you care about power, the world is heterogeneous?

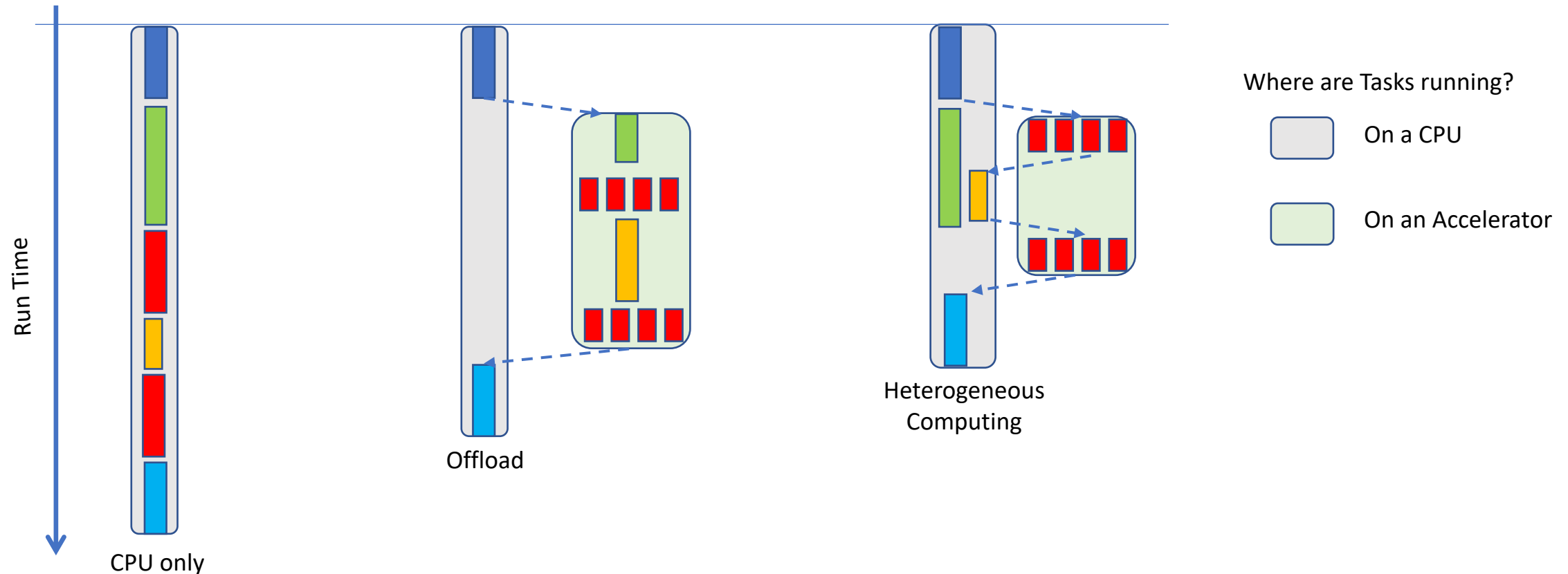
Specialized processors doing operations suited to their architecture are more efficient than general purpose processors.



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

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 (<u>optimized by Intel</u>)	<i>“Simulated”</i> 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	205.6
K-means (single iteration)	148	2	7.1	7.1
KNN	154	62	59.8	59.8
UMAP	2571	21	84.5	84.5
Louvain clustering	1153	2.4	6.0	6.0
Leiden clustering	6345	1.7	28.4	28.4
Reanalysis of subgroup	255	17.9	22.5	22.5
Rest	39	49.2	49.0	49.0
End-to-End runtime	18338	686	483.6	211.5

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.

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 μ s 10 Gbps flash	People to people
Fifth 2015	Per socket wall ... accelerators take off	Machine Learning, data centric computing	10 μ s 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

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 **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

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.


Cloud

- ~~X.~~ ~~The network is reliable~~
- ~~X.~~ ~~Latency is **low and fixed**~~
- ~~X.~~ ~~Bandwidth is **high and fixed**~~
- ~~X.~~ ~~The network is secure~~
- ~~X.~~ ~~Topology doesn't change~~
- ~~X.~~ ~~There is one administrator~~
- ~~X.~~ ~~Transport cost is **negligible**~~
- ~~X.~~ ~~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
- ~~X.~~ ~~Transport cost is **negligible**~~
- ✓8. The network is homogeneous

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.

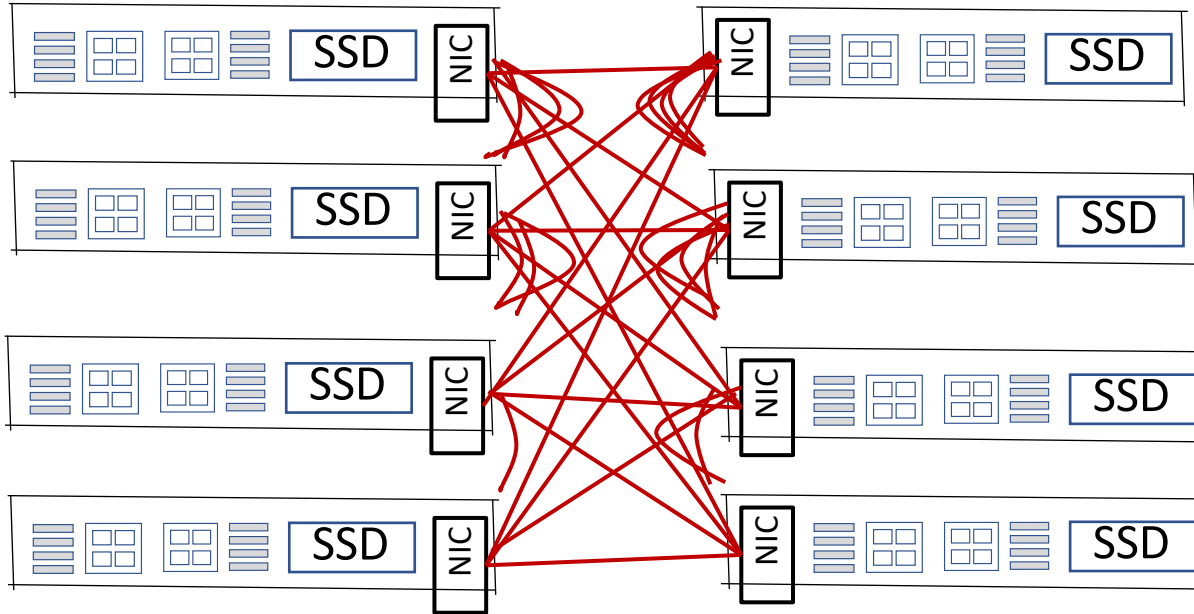
An impenetrable wall separates them from the cloud-native world

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 μ s 10 Gbps flash	People to people
Fifth 2015	Per socket wall ... accelerators take off	Machine Learning, data centric computing	10 μ s 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)

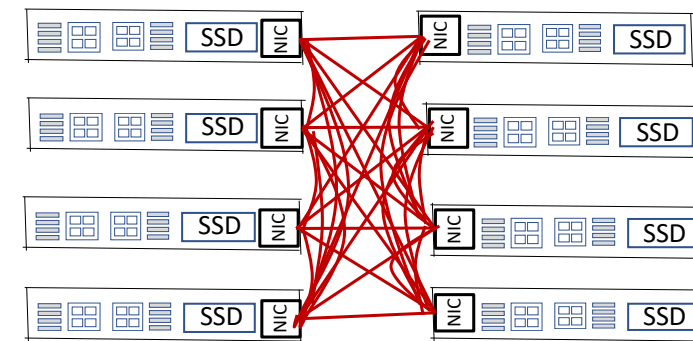
Read 1 MB bytes sequentially from SSD 500,000 ns (500 us)

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)



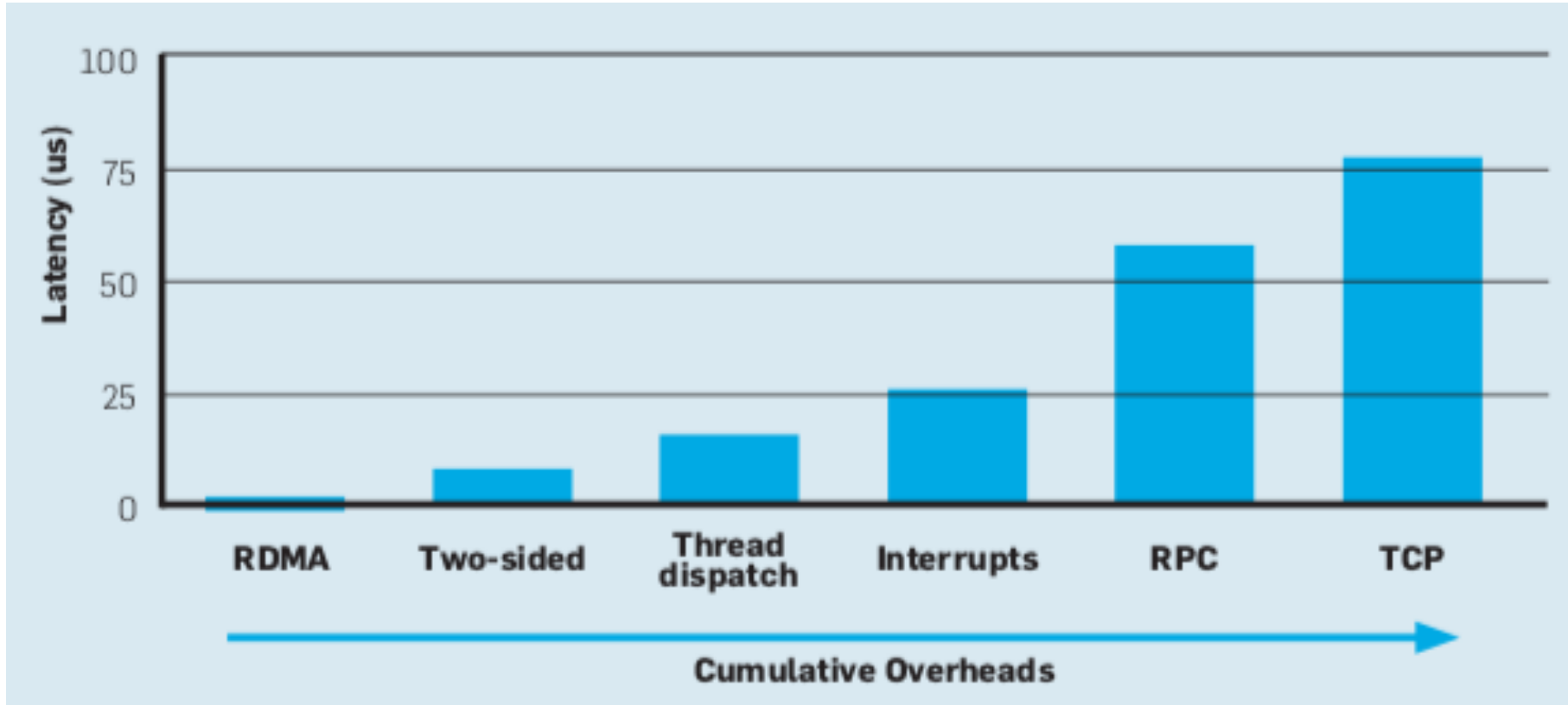
A cluster of nodes with a Clique network topology and low latency optical network...

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.

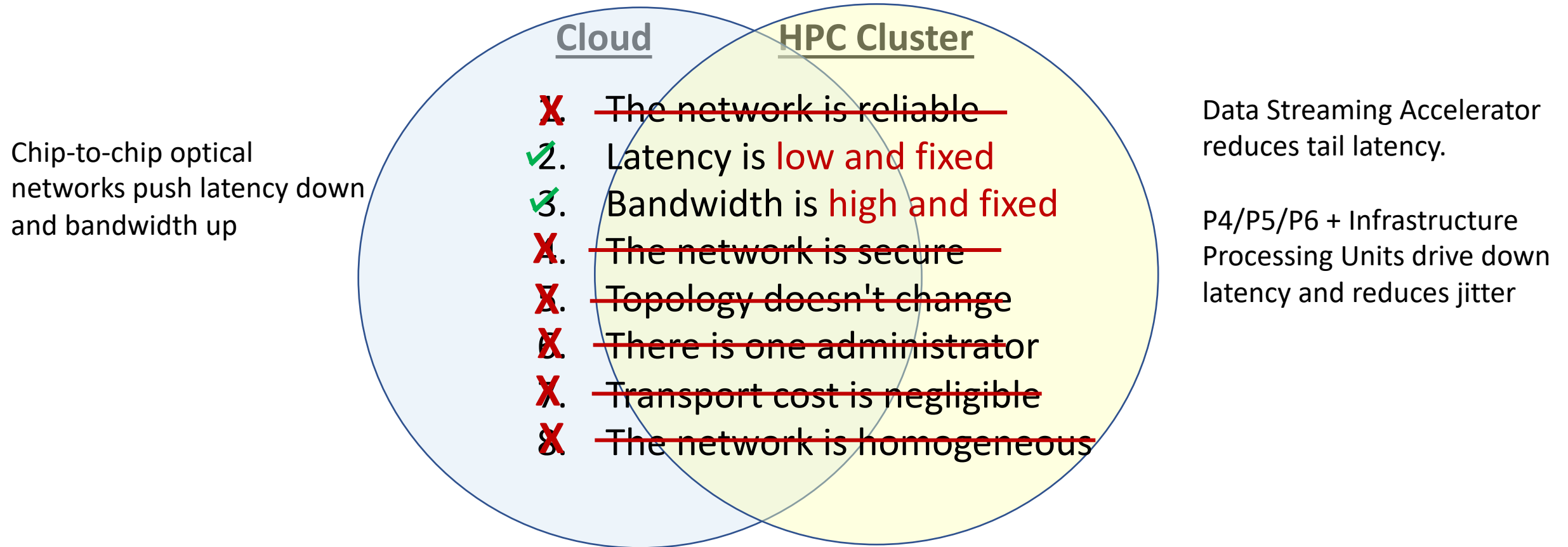
Take out the big stuff & you're left with lots of μ s overheads

All those SW overheads add up ... like bricks that combine to build a networking-wall ... turning a 2 μ s network into a 100 μ s 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 $O(\mu$ s) latencies.

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



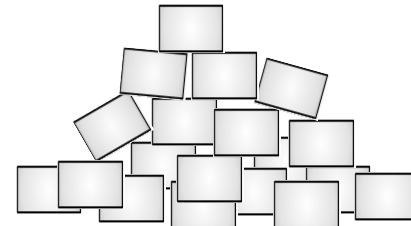
With Low Latencies, high bandwidths and stable performance, we can do loosely synchronous and synchronous applications in the cloud. The economics of the cloud vs dedicated HPC clusters means the cloud will dominate HPC

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

The three domains of parallel programming

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Memory	Single Address Space	Distributed memory, local memory owned by individual processes	Distributed object store (in memory) backed by a persistent storage system
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Advances in networking technology plus low-overhead software stacks optimized to reduce tail-latency will shatter this wall



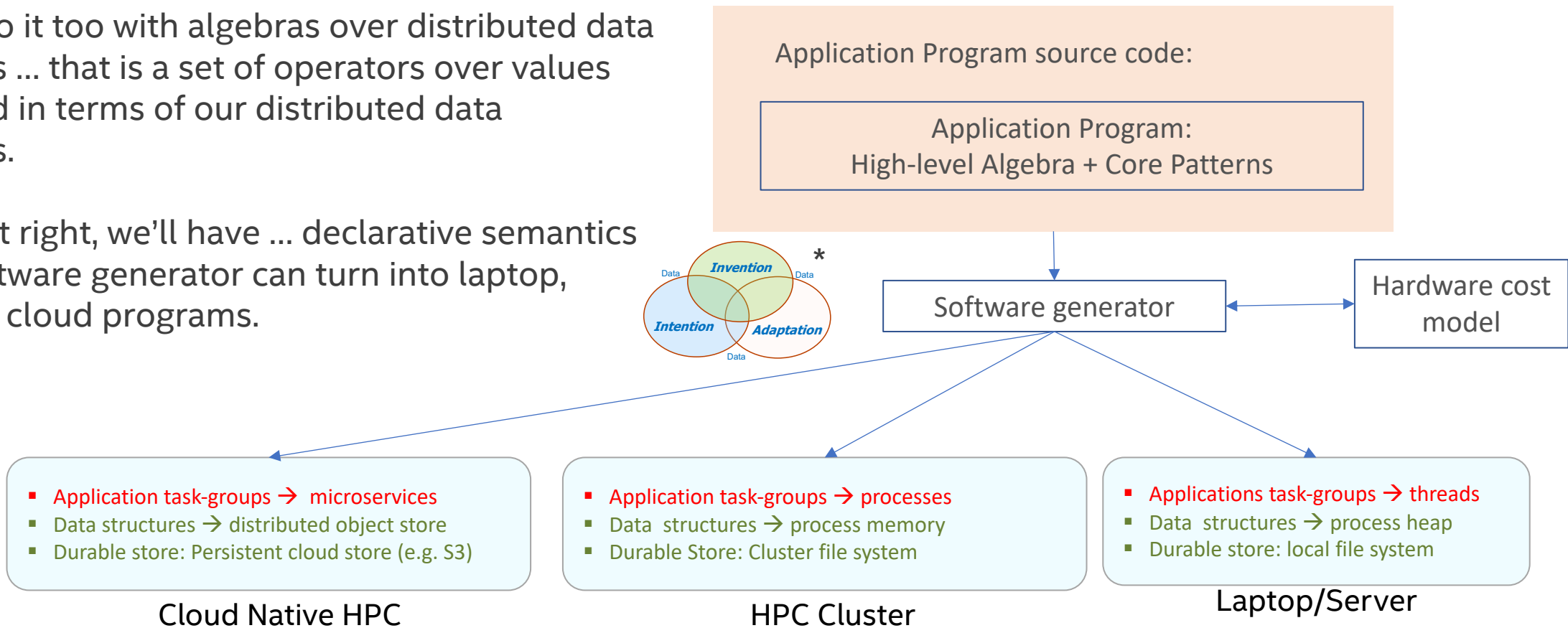
The three domains of parallel programming

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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.

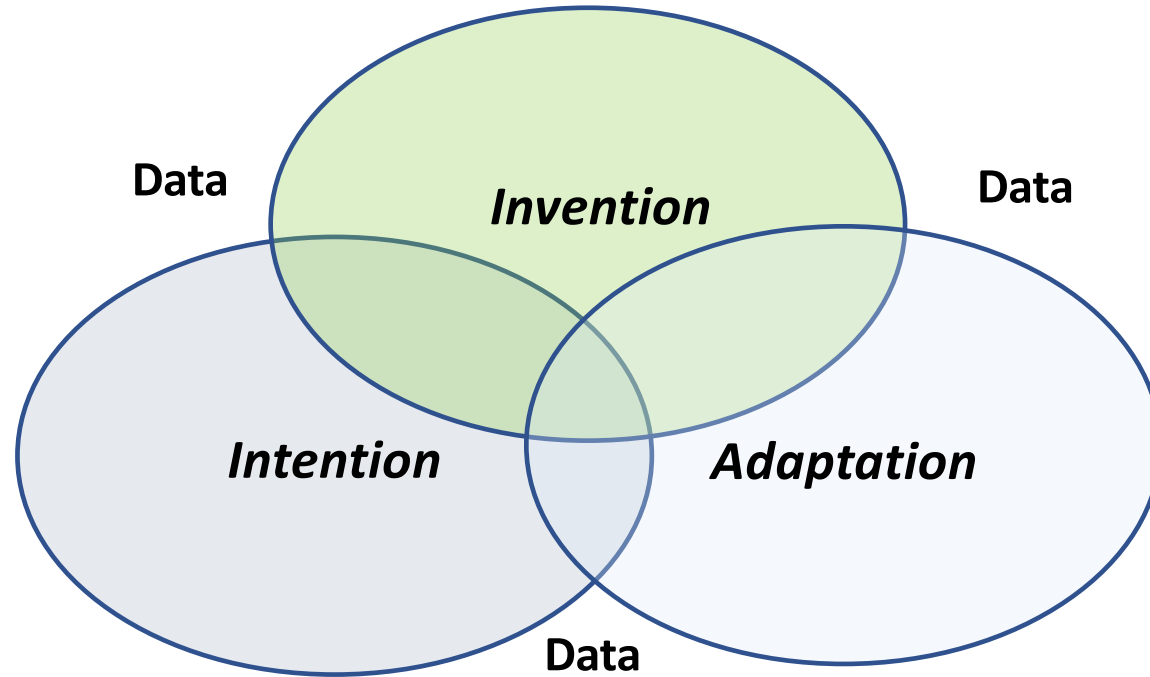
One codebase → many systems

- 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)



Justin Gottschlich, Intel Labs
Armando Solar-Lezama, MIT
Nesime Tatbul, Intel Labs
Michael Carbin, MIT
Martin Rinard, MIT
Regina Barzilay, MIT
Saman Amarasinghe, MIT
Joshua B Tenenbaum, MIT
Tim Mattson, Intel Labs

- **MP is the automation of software development**

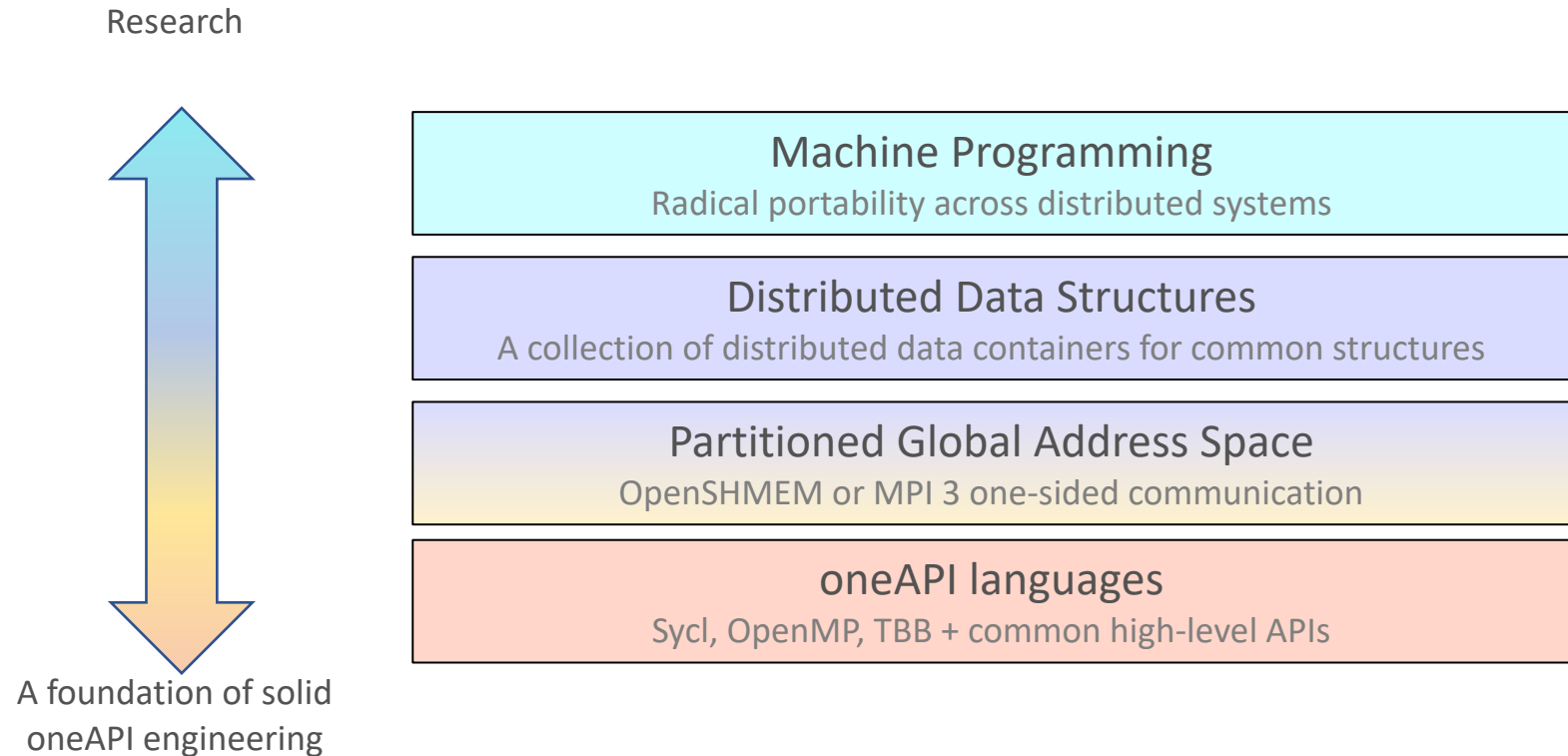
- **Intention:** Discover the intent of a programmer
- **Invention:** Create new algorithms and data structures
- **Adaptation:** Evolve in a changing hardware/software world

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 heterogeneous 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.