OpenMP* GPU Offload Basics

Objectives

- To learn the basic OpenMP* offload constructs to deploy OpenMP application for execution on GPUs

- Prerequisites
  - Knowledge of using OpenMP with Fortran, C or C++ on CPUs

Agenda

- oneAPI and OpenMP* Offload
- OpenMP on CPUs Review
- Introduction to OpenMP Offload
- Constructs to Manage Device Data
- Constructs to Leverage Parallelism
- Case Study
- Summary

oneAPI and OpenMP* Offload

intel®

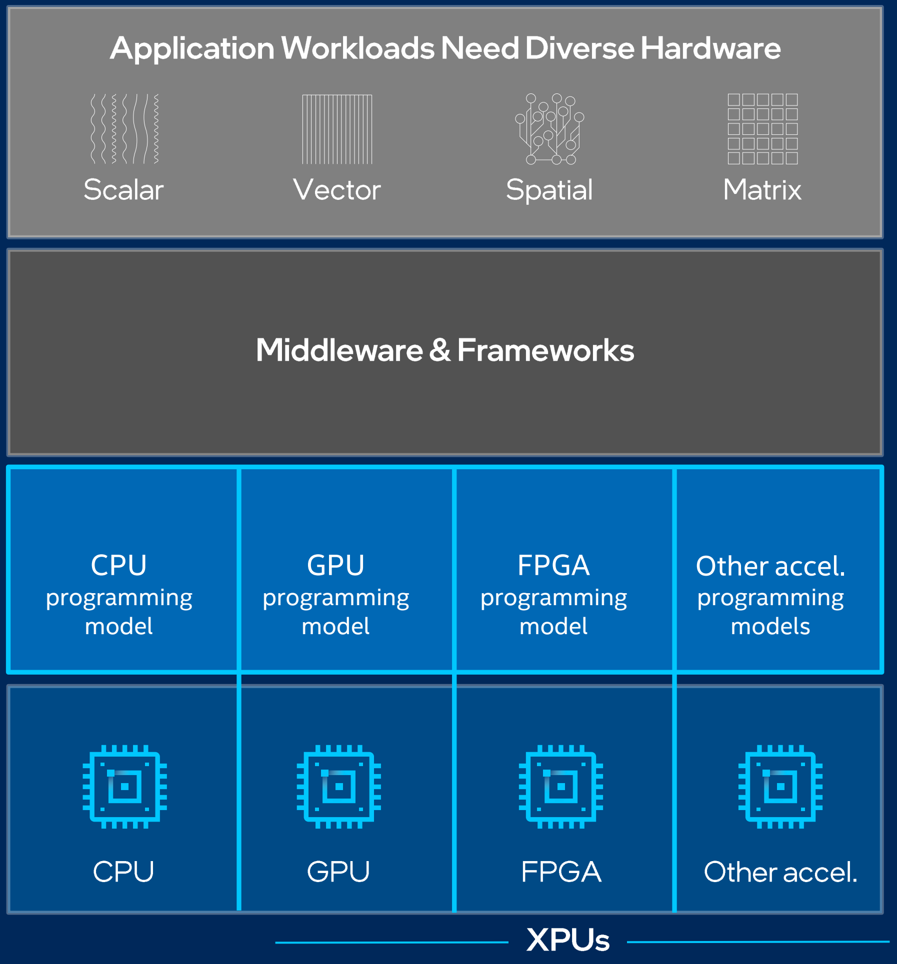
Programming Challenges
for Multiple Architectures

Growth in specialized workloads

Variety of data-centric hardware required

Separate programming models and toolchains for each architecture are required today

Software development complexity limits freedom of architectural choice



oneAPI

One Programming Model for Multiple Architectures and Vendors

Freedom to Make Your Best Choice

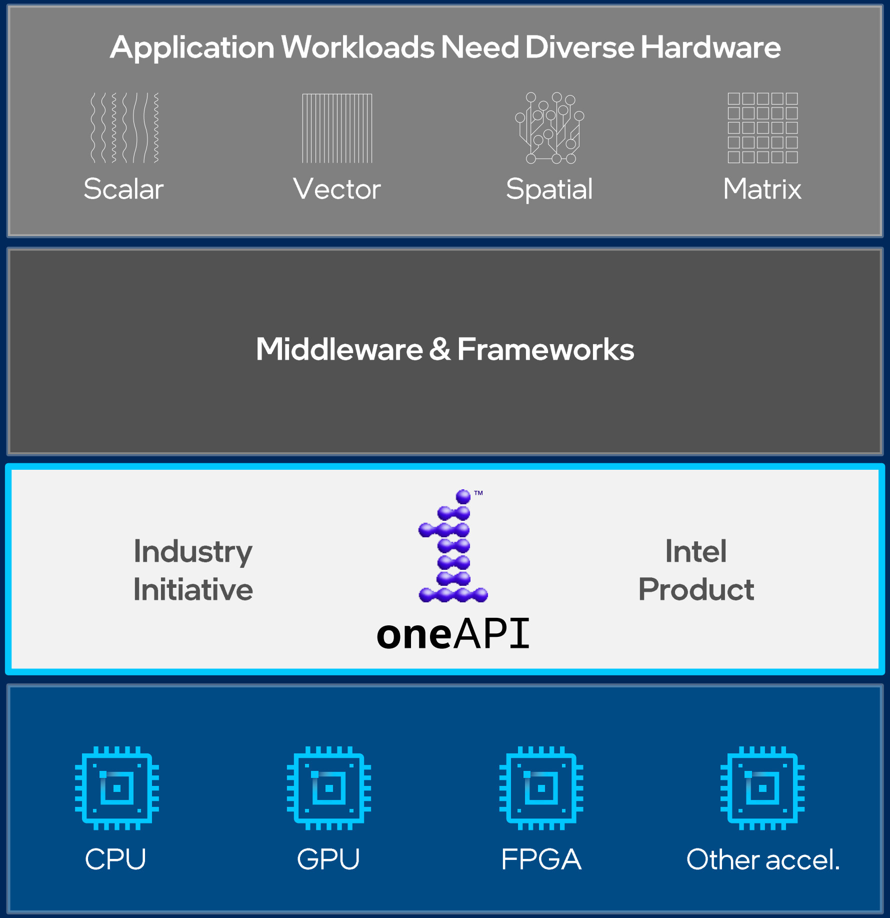
- Choose the best accelerated technology the software doesn't decide for you

Realize all the Hardware Value

- Performance across CPU, GPUs, FPGAs, and other accelerators

Develop & Deploy Software with Peace of Mind

- Open industry standards provide a safe, clear path to the future
- Compatible with existing languages and programming models including C++, Python, SYCL, OpenMP, Fortran, and MPI

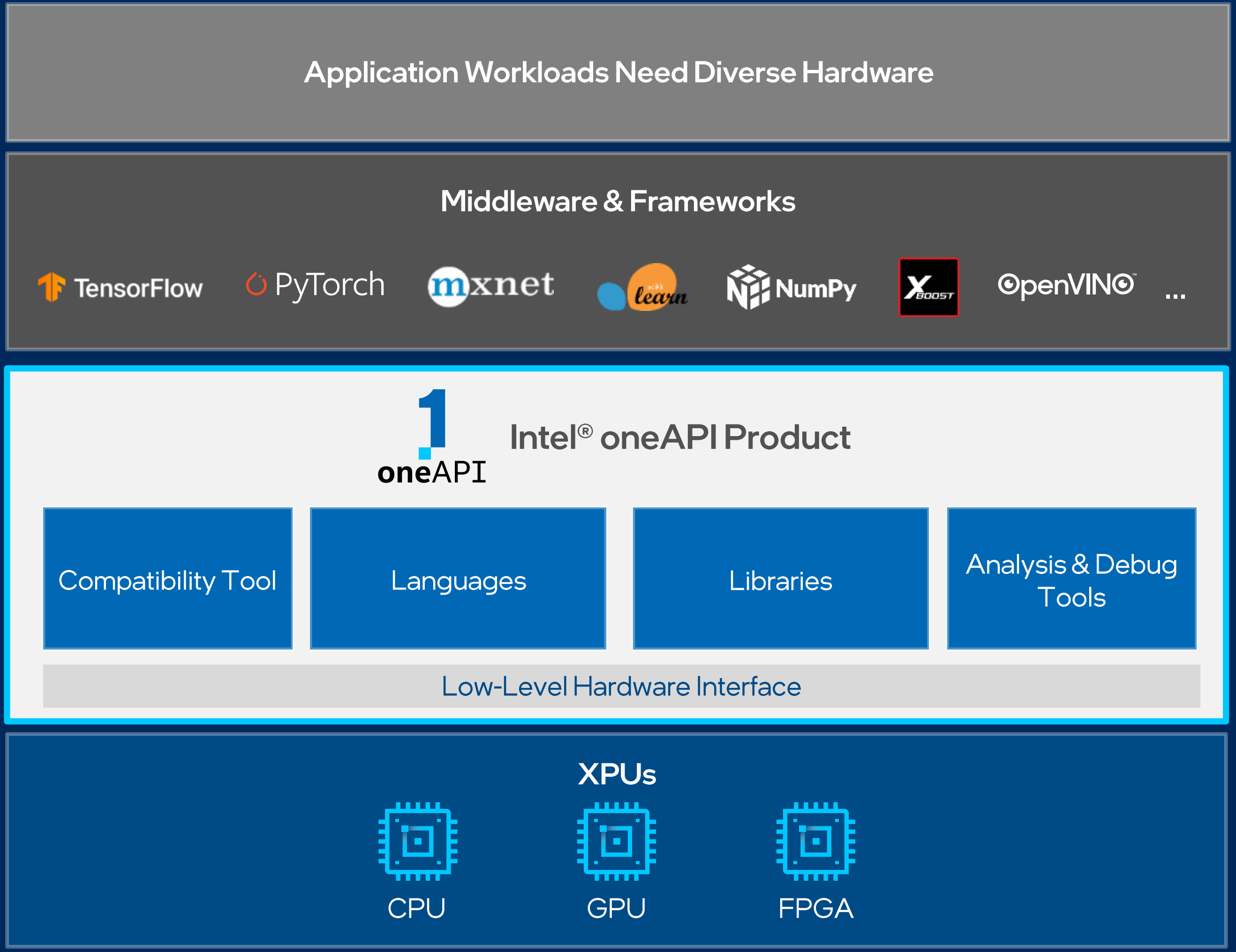


Intel® oneAPI Product

Built on Intel's Rich Heritage of CPU Tools Expanded to XPUs

A complete set of advanced compilers, libraries, and porting, analysis and debugger tools

- Accelerates compute by exploiting cutting-edge hardware features
- Interoperable with existing programming models and code bases (C++, Fortran, Python, OpenMP, etc.), developers can be confident that existing applications work seamlessly with oneAPI
- Eases transitions to new systems and accelerators—using a single code base frees developers to invest more time on innovation



Available Now

Visit software.intel.com/oneapi for more details
Some capabilities may differ per architecture and custom-tuning will still be required. Other accelerators to be supported in the future.

Intel® oneAPI Toolkits

A complete set of proven developer tools expanded from CPU to XPU

Intel® oneAPI **Base** Toolkit

Native Code Developers

A core set of high-performance tools for building C++, Data Parallel C++ applications & oneAPI library-based applications

Add-on **Domain-specific** Toolkits

Specialized Workloads

Intel® oneAPI Tools for HPC

Deliver fast Fortran, OpenMP & MPI applications that scale

Intel® oneAPI Tools for IoT

Build efficient, reliable solutions that run at network's edge

Intel® oneAPI AI Analytics Toolkit

Accelerate machine learning & data science pipelines with optimized DL frameworks & high-performing Python libraries

Intel® oneAPI Rendering Toolkit

Create performant, high-fidelity visualization applications

Toolkit **powered by oneAPI**

Data Scientists & AI Developers

Intel® Distribution of OpenVINO™ Toolkit

Deploy high performance inference & applications from edge to cloud

Intel® oneAPI Tools for HPC

Intel® oneAPI HPC Toolkit

Deliver Fast Applications that Scale

What is it?

A toolkit that adds to the Intel® oneAPI Base Toolkit for building high-performance, scalable parallel code on C++, Fortran, OpenMP & MPI from enterprise to cloud, and HPC to AI applications.

Who needs this product?

- OEMs/ISVs
- C++, Fortran, OpenMP, MPI Developers

Why is this important?

- Accelerate performance on Intel® Xeon® & Core™ Processors and Intel® Accelerators
- Deliver fast, scalable, reliable parallel code with less effort built on industry standards

Learn More: intel.com/oneAPI-HPCKit

Intel® oneAPI Base & HPC Toolkits

Direct Programming

- Intel® C++ Compiler Classic
- Intel® Fortran Compiler Classic
- Intel® Fortran Compiler (Beta)
- Intel® oneAPI DPC++/C++ Compiler
- Intel® DPC++ Compatibility Tool
- Intel® Distribution for Python
- Intel® FPGA Add-on for oneAPI Base Toolkit

API-Based Programming

- Intel® MPI Library
- Intel® oneAPI DPC++ Library oneDPL
- Intel® oneAPI Math Kernel Library - oneMKL
- Intel® oneAPI Data Analytics Library - oneDAL
- Intel® oneAPI Threading Building Blocks - oneTBB
- Intel® oneAPI Video Processing Library - oneVPL
- Intel® oneAPI Collective Communications Library oneCCL
- Intel® oneAPI Deep Neural Network Library - oneDNN
- Intel® Integrated Performance Primitives – Intel® IPP

Analysis & debug Tools

- Intel® Inspector
- Intel® Trace Analyzer & Collector
- Intel® Cluster Checker
- Intel® VTune™ Profiler
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Intel® oneAPI **HPC** Toolkit +
Intel® oneAPI **Base** Toolkit

OpenMP* on CPUs

*Other names and brands may be claimed as the property of others.

OpenMP* Overview

- Cross-platform standard supporting shared-memory-multi-processing programming in C, C++ and Fortran
  - API for writing multithreaded applications
  - Set of compiler directives and library routines for parallel application programmers
  - Greatly simplifies writing multi-threaded programs in Fortran, C and C++
  - Portable across vendors and platforms
  - Supports various types of parallelism

OpenMP* History

- 1997: Version 1.0 for Fortran
- 1998: Version 1.0 for C/C++
- 2002-2005: Versions 2.0-2.5, Merger of Fortran and C/C++ specifications
- 2008: Version 3.0, Incorporates Task Parallelism
- 2013: Version 4.0, Support for Accelerators, SIMD support
- 2018: Version 5.0, C11/C++17/Fortran 2008 support

OpenMP* Threads

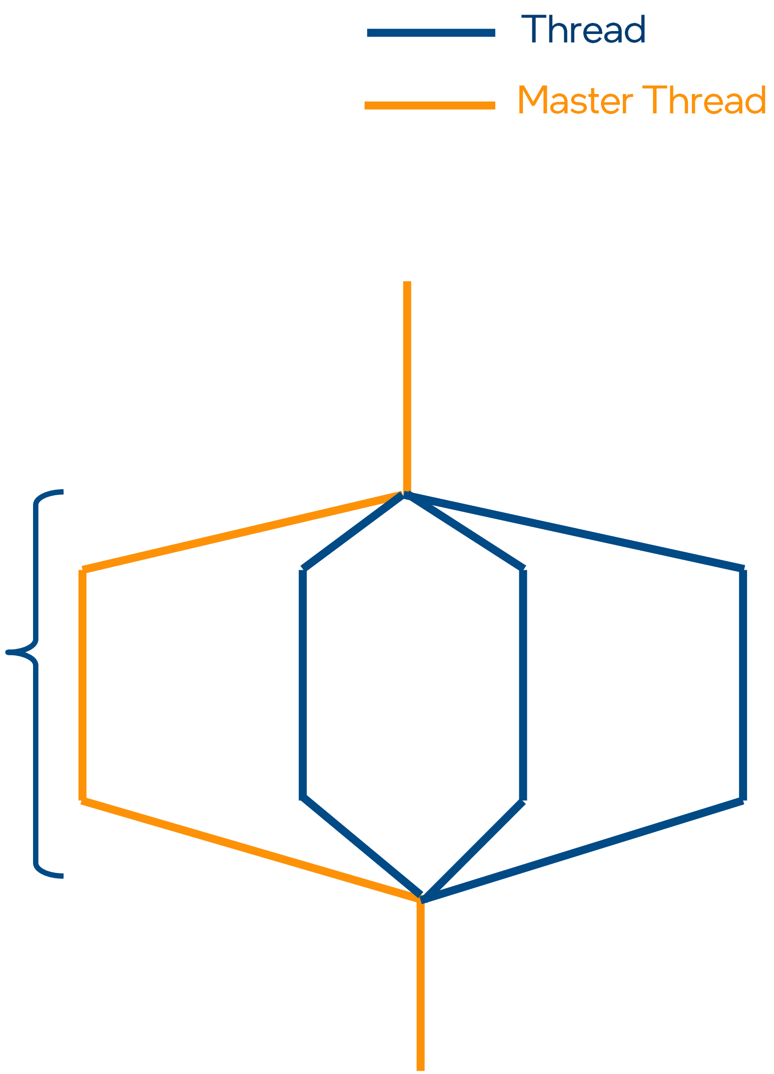
- Create threads with the **parallel** construct

```
#include <omp.h>

void saxpy()
{
   float a, x[ARRAY_SZ], y[ARRAY_SZ];
#pragma omp parallel
{
   int id=omp_get_thread_num();
   int nthrs=omp_get_num_threads();
   for (int i=id; i < ARRAY_SZ; i+=nthrs) {
      y[i] = a * x[i] + y[i];
   }
}
}
```

Parallel Region.

Team of threads created.

Each thread executes the same code redundantly



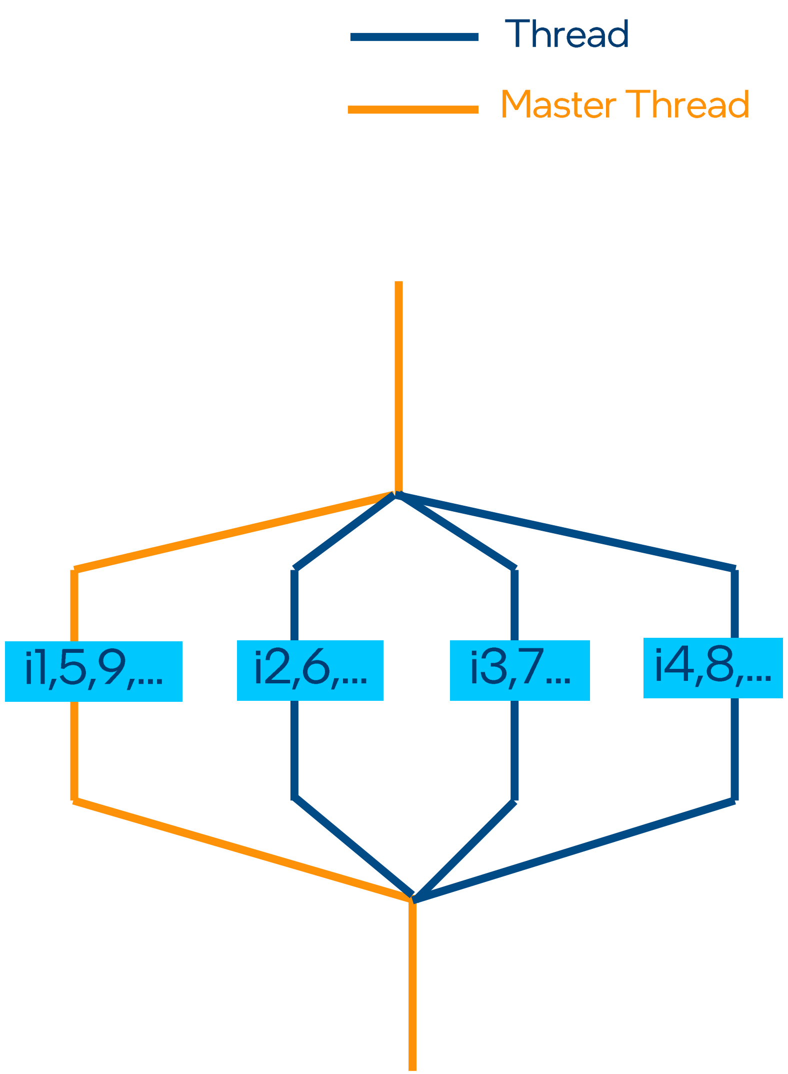
Loops

- Use For/Do Loop Directive to Workshare

```
#include <omp.h>

void saxpy()
{
   float a, x[ARRAY_SZ], y[ARRAY_SZ];
#pragma omp parallel
{
#pragma omp for
   for (int i=0; i < ARRAY_SZ; i++) {
      y[i] = a * x[i] + y[i];
   }
}
}
```

Workshare:

Distributes the execution of loop iterations across the threads



Basic Examples

C/C++

```
#include <omp.h>

…
#pragma omp parallel for reduction (+:sum)
{
   for (int i=0; i<ARRAY_SZ; i++) {
      sum += x[i];
   }
}
…
```

Fortran

```
program main
   use omp_lib
   …
   !$omp parallel do reduction (+:total)
   do i=0,ARRAY_SZ
      total = total + x(i)
   end do
   !$omp end parallel do
…
end program main
```

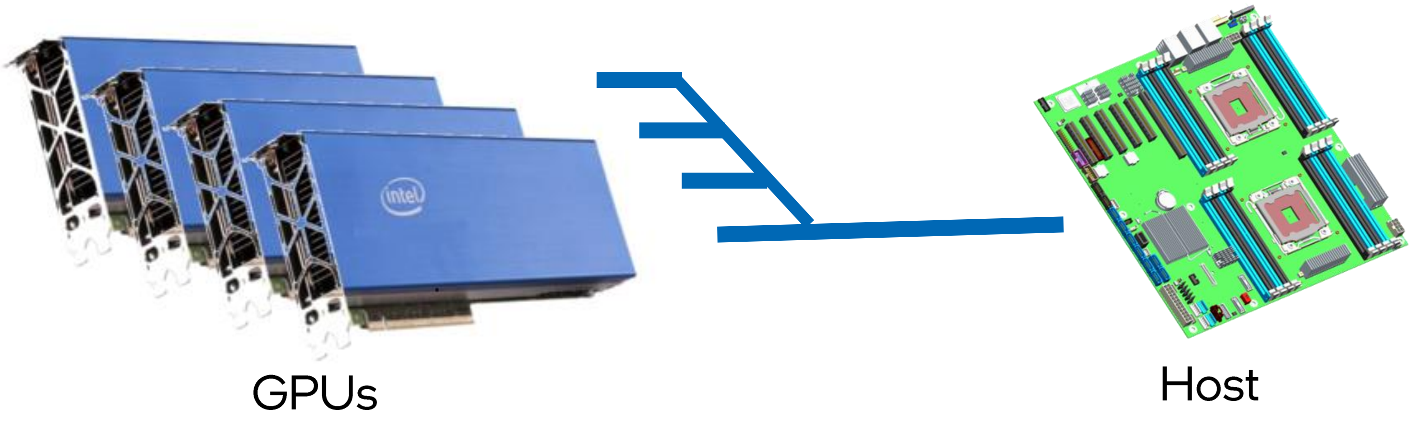
Other Notable OpenMP* Constructs

- Sections/Section
  - Distribute blocks of code (sections) among existing threads
- Task
  - Create independent units of work (including code, data, and internal control variables) for execution on a thread
- SIMD
  - Specifies iterations of a given loop can be executed concurrently with SIMD instructions
    - i.e. compiler can ignore vector dependencies

Introduction: OpenMP* Offload

OpenMP* Device Model

- OpenMP 4.0+ supports accelerators/coprocessors (devices)
  - Not GPU-specific
- Device model:
  - One host
  - Multiple accelerators/coprocessors of the **same** kind



OpenMP* Offload Compiler Support

- OpenMP Offload Supported in the Intel® oneAPI HPC Toolkit
  - Need to enable OpenMP* 4.5 support (-fiopenmp) and OpenMP* 4.5 offloading support (-fopenmp-targets=spir64)
  - Intel® oneAPI C++ Compiler

```
icx –fiopenmp –fopenmp-targets=spir64 <source>.c

icpx –fiopenmp –fopenmp-targets=spir64 <source>.cpp
```

  - Intel® Fortran Compiler

```
ifx –fiopenmp –fopenmp-targets=spir64 <source>.f90
```

OpenMP* 4.0 for Devices - Constructs

- target construct transfer control and data from the host to the device
- Syntax (C/C++)

```
#pragma omp target [clause[[,] clause],…]
structured-block
```

- Syntax (Fortran)

```
!$omp target [clause[[,] clause],…]
structured-block
!$omp end target
```

- Clauses

```
device(scalar-integer-expression)
map([{alloc | to | from | tofrom}:] list)
if(scalar-expr)
```

Execution Model

- The `target` construct transfers the control flow to the target device
  - Transfer of control is sequential and synchronous
  - The transfer clauses control direction of data flow
  - Array notation is used to describe array length

Target Region Example: saxpy

Sequential Host Code

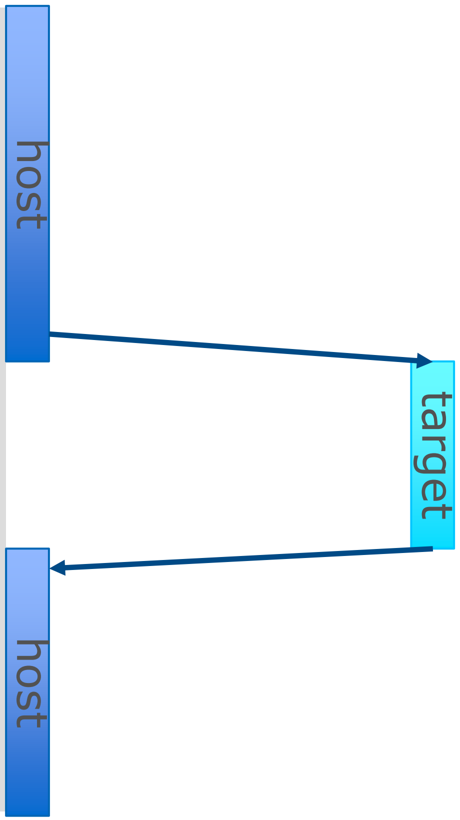
```
void saxpy() {
    float a, x[ARRAY_SZ], y[ARRAY_SZ];
    double t = 0.0;
    double tb, te;
    tb = omp_get_wtime();
```

Target Region

```
#pragma omp target
    for (int i = 0; i < ARRAY_SZ; i++) {
        y[i] = a * x[i] + y[i];
    }
```

Sequential Host Code

```
    te = omp_get_wtime();
    t = te - tb;
    printf("Time of kernel: %lf\n", t);
}
```




```
icx -fiopenmp -fopenmp-targets=spir64 -o saxpy saxpy.c
```

Device Clause

- Specify which device to offload to in a multi-device environment

```
#pragma omp target device(i)
```

  - Device number an integer
    - Assignment is implementation-specific
    - Usually start at 0 and sequentially increments
  - Works with **`target, target data, target enter/exit data, target update`** directives

Calling Functions Inside Target Area

- **`declare target`** construct compiles a version of the function/subroutine for the target device
  - Function compiled for both host execution and target execution by default

```
#pragma omp declare target
int devicefunc(){
…
}
#pragma omp end declare target

#pragma omp target
{
          result = devicefunc();
}
```

```
subroutine devicefunc()
!$omp declare target device_type(device)
…
end subroutine

program main
!$omp target
          call devicefunc()
!$omp end target
end program
```

Optional device_type specifies host and/or device execution

if device is specified, it needs to be always available

Managing Device Data

Offload Data

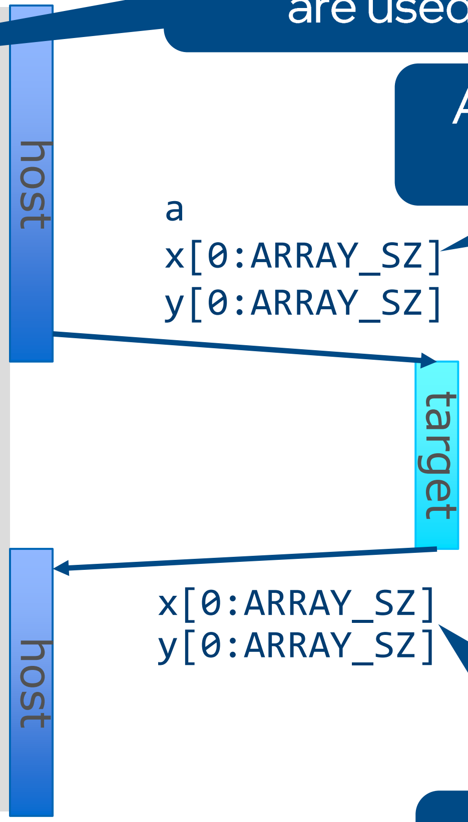
- Host and devices have separate memory spaces
  - Data needs to be mapped to the target device in order to be accessed inside the target region
  - Default for variables accessed inside the target region:
    - Scalars: treated as firstprivate
    - Static arrays: copied to and from the device on entry and exit
  - Data environment is lexically scoped
    - Data environment is destroyed at closing curly brace
    - Allocated buffers/data are automatically released

Example: saxpy

```
void saxpy() {
    float a, x[ARRAY_SZ], y[ARRAY_SZ];
    double t = 0.0;
    double tb, te;
    tb = omp_get_wtime();
#pragma omp target
    for (int i = 0; i < ARRAY_SZ; i++) {
        y[i] = a * x[i] + y[i];
    }
    te = omp_get_wtime();
    t = te - tb;
    printf("Time of kernel: %lf\n", t);
}
```

The compiler identifies variables that are used in the `target` region.

All accessed arrays are copied from host to device and back



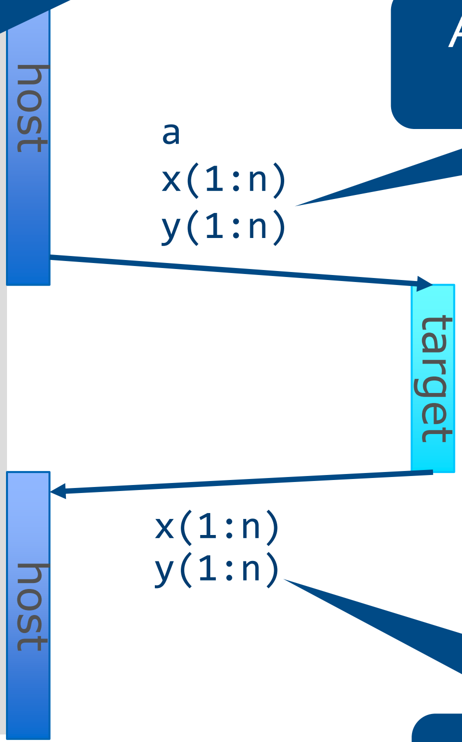
Copying x back is not necessary: it was not changed.

```
icx -fiopenmp -fopenmp-targets=spir64 -o saxpy saxpy.c
```

Example: saxpy

The compiler identifies variables that are used in the `target` region.

```
subroutine saxpy(a, x, y, n)
    use iso_fortran_env
    integer :: n, i
    real(kind=real32) :: a
    real(kind=real32), dimension(n) :: x
    real(kind=real32), dimension(n) :: y

!$omp target
    do i=1,n
        y(i) = a * x(i) + y(i)
    end do
!$omp end target
end subroutine
```



All accessed arrays are copied from host to device and back

Copying x back is not necessary: it was not changed.

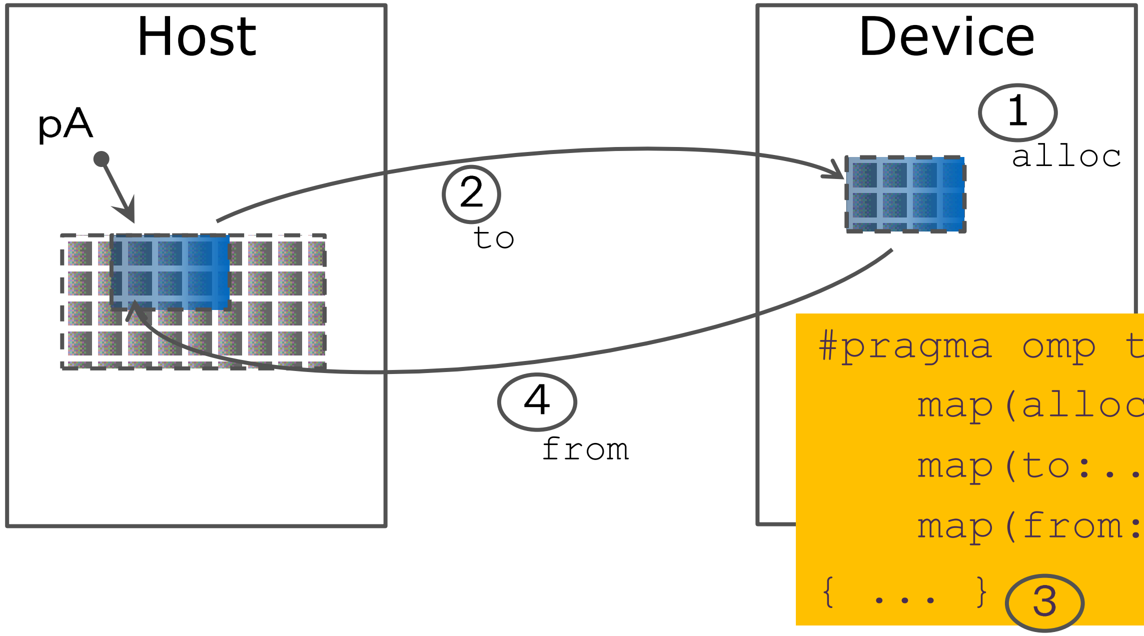
```
ifx -fiopenmp -fopenmp-targets=spir64 -o saxpy saxpy.f90
```

Map Clause

- Use **`map`** clause to manually determine how an original variable in a data environment is mapped to a corresponding variable in a device data environment
  - `omp target map (`*`map-type: list`*`)`
  - Available map-type
    - alloc : allocate storage for variable on target device (values not copied)
    - to : alloc and assign value of original variable on target region entry
    - from : alloc and assign value to original variable on target region exit
    - tofrom: default, both to and from

Map Clause

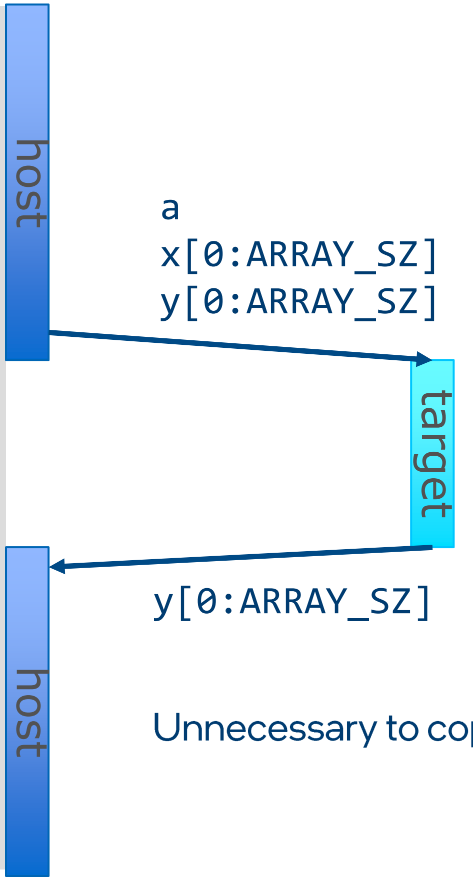
- Use **`map`** clause to manually determine how an original variable in a data environment is mapped to a corresponding variable in a device data environment




```
#pragma omp target \
    map(alloc:...) \
    map(to:...) \
    map(from:...)
{ ... }
```

Example: saxpy

```
void saxpy() {
    double a, x[ARRAY_SZ], y[ARRAY_SZ];
    double t = 0.0;
    double tb, te;
    tb = omp_get_wtime();
#pragma omp target map(to:x) \
                   map(tofrom:y)
    for (int i = 0; i < ARRAY_SZ; i++) {
        y[i] = a * x[i] + y[i];
    }
    te = omp_get_wtime();
    t = te - tb;
    printf("Time of kernel: %lf\n", t);
}
```



Unnecessary to copy x back to the host

```
icx -fiopenmp -fopenmp-targets=spir64 -o saxpy saxpy.c
```

Mapping Dynamically Allocated Data

- When pointers are dynamically allocated, number of elements to be mapped must be explicitly specified

```
#pragma omp target map(to:array[start:length])
```

```
!$omp target map(to:array(start:end))
```

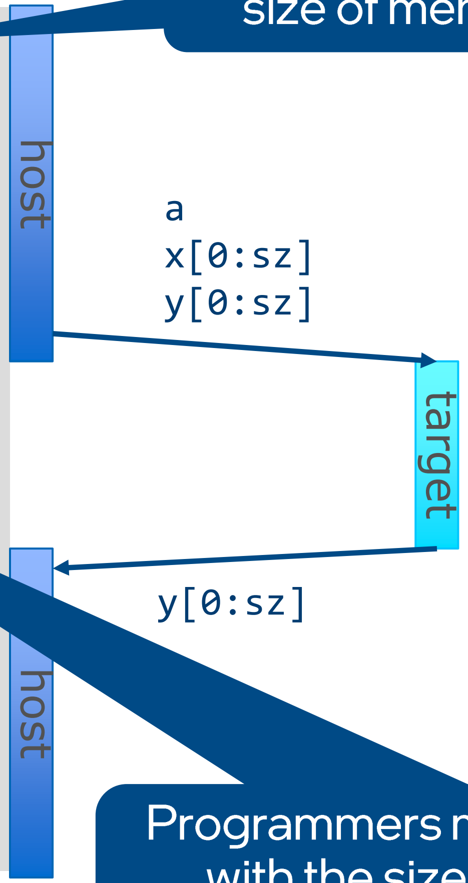
  - Partial array may be specified
  - Note: syntax in C/C++ (uses *length*) is different from Fortran (uses *end*)

Example: saxpy

```
void saxpy(float a, float* x, float* y,
           int sz) {
    double t = 0.0;
    double tb, te;
    tb = omp_get_wtime();
#pragma omp target map(to:x[0:sz]) \
                   map(tofrom:y[0:sz])
    for (int i = 0; i < sz; i++) {
        y[i] = a * x[i] + y[i];
    }
    te = omp_get_wtime();
    t = te - tb;
    printf("Time of kernel: %lf\n", t);
}
```

```
icx -fiopenmp -fopenmp-targets=spir64 -o saxpy saxpy.c
```

The compiler cannot determine the size of memory behind the pointer.



Programmers must help the compiler with the size of the data transfer needed.

Minimize Data Copy Across Target Regions

- Use **`target data`**, **`target enter data`**, and **`target exit data`** to form target data region and optimize sharing of data between host and device
  - Maps variables, code execution not offloaded
  - Variables remain on device for duration of the target data region
  - **`target update`** construct can copy values between host and device

`target data` Construct Syntax

- Create scoped data environment and transfer data from the host to the device and back
- Syntax (C/C++)

```
#pragma omp target data [clause[[,] clause],…]
structured-block
```

- Syntax (Fortran)

```
!$omp target data [clause[[,] clause],…]
structured-block
!$omp end target data
```

- Clauses

```
device(scalar-integer-expression)
map([{alloc | to | from | tofrom | release | delete}:] list)
if(scalar-expr)
```

Target Data Example

- Use target data construct to create target data environment

```
#pragma omp target data map(tofrom: x)
{
        #pragma omp target map(to: y)
        {
                ...//1st target region, device operations on x and y
        }
        host_update(y);
        #pragma omp target map(to: y)
        {
                ...//2nd target region, device operations on x and y
        }
}
```

Device data environment created, array x is mapped

y must be mapped at each target region since it's updated by the host here

`target update` Construct Syntax

- Issue data transfers to or from existing data device environment
- Syntax (C/C++)

  ```
  #pragma omp target update [clause[[,] clause],…]
  ```

  Syntax (Fortran)

  ```
  !$omp target update [clause[[,] clause],…]
  ```

  Clauses

  ```
  device(scalar-integer-expression)
  to(list)
  from(list)
  if(scalar-expr)
  ```

Target Enter/Exit Data and Update Example

- Use **`target enter/exit data`** to map to/from target data environment
- Use **`target update`** to maintain consistency between host and device

```
#pragma omp target enter data map(to: y) map(alloc: x)
#pragma omp target
{         ...//1st target region, device operations on x and y
}
#pragma omp target update from(y)
host_update(y);
#pragma omp target update to(y)

#pragma omp target
{         ...//2nd target region, device operations on x and y
}
#pragma omp target exit data map(from:x)
```

Unstructured mapping, data environment can span multiple functions

y must be updated from and to the device since it's updated by the host here

Map Global Variable to Device

- Use **`declare target`** construct for to map variables to the device for the duration of the program

```
#pragma omp declare target
int a[N]
#pragma omp end declare target
…
init(a);
#pragma omp target update to(a)
…
#pragma omp target teams\
distribute parallel for
for (int i=0; i<N; i++){
         result[i] = process(a[i]);
}
```

```
module my_arrays
!$omp declare target (a)
integer :: a(N)
end module
…
use my_arrays
integer :: i
call init(a);
!$omp target update to(a)
…
!$omp target teams distribute &
!$omp&       parallel do
do i=1,N
         result(i) =
process(a(i));
end do
```

Unified Shared Memory

- Single address space for CPU and GPU
- Data migration among CPU and GPUs transparent to the application
  - Explicit mapping of data not required

Type	Location	Accessible From	Allocation Routine
Host	Host	Host or Device	omp_target_alloc_host(size, device_num)
Device	Device	Device	omp_target_alloc_device(size, device_num)
Shared	Host or Device	Host or Device	omp_target_alloc_shared(size, device_num)

- Use Shared or Host memory for implicit data movement to achieve ease of coding
- Use Device memory for explicit data movement to achieve maximum performance

Unified Shared Memory (Implicit) Example

```
#include <stdio.h>
#include <stdlib.h>
#include <omp.h>
#define SIZE 1024
#pragma omp requires unified_shared_memory
int main() {
  int deviceId = (omp_get_num_devices() > 0) ?
       omp_get_default_device() : omp_get_initial_device();
  int *a = (int *)omp_target_alloc_shared(SIZE * sizeof(int) , deviceId);
  int *b = (int *)omp_target_alloc_shared(SIZE * sizeof(int) , deviceId);
  for (int i = 0; i < SIZE; i++) {
    a[i] = i;     b[i] = SIZE - i;
  }
#pragma omp target teams distribute parallel for
  for (int i = 0; i < SIZE; i++) {
    a[i] += b[i];
  }

  for (int i = 0; i < SIZE; i++) {
    if (a[i] != SIZE) {
      printf("%s failed\n", __func__);
      return EXIT_FAILURE;
    }
  }
  omp_target_free(a, deviceId);
  omp_target_free(b, deviceId);
  printf("%s passed\n", __func__);
  return EXIT_SUCCESS;
}
```

USM support via managed memory allocator

Unified Shared Memory (Explicit) Example

```
…
int main() {
  int deviceId = (omp_get_num_devices() > 0) ? omp_get_default_device() : omp_get_initial_device();
  int *a = (int *)malloc(SIZE * sizeof(int));  int *b = (int *)malloc(SIZE * sizeof(int));
  for (int i = 0; i < SIZE; i++) {
    a[i] = i;     b[i] = SIZE - i;
  }
 int *a_dev = (int *)omp_target_alloc_device(SIZE * sizeof(int) , deviceId);
 int *b_dev = (int *)omp_target_alloc_device(SIZE * sizeof(int) , deviceId);
 int error=omp_target_memcpy(a_dev, a, SIZE*sizeof(int), 0, 0, deviceId, 0);
 error=omp_target_memcpy(b_dev, b, SIZE*sizeof(int), 0, 0, deviceId, 0);
 #pragma omp target teams distribute parallel for
  for (int i = 0; i < SIZE; i++) {
    a[i] += b[i];
  }
 error=omp_target_memcpy(a, a_dev, SIZE*sizeof(int), 0, 0, 0, deviceId);
 error=omp_target_memcpy(b, b_dev, SIZE*sizeof(int), 0, 0, 0, deviceId);

  for (int i = 0; i < SIZE; i++) {
    if (a[i] != SIZE) { printf("%s failed\n", __func__);  return EXIT_FAILURE; }}
 omp_target_free(a_dev, deviceId);
 omp_target_free(b_dev, deviceId);
  free(a);  free(b);
  printf("%s passed\n", __func__);
  return EXIT_SUCCESS;
}
```

Explicit Data Movement from Host to Device

Explicit Data Movement from Device to Host

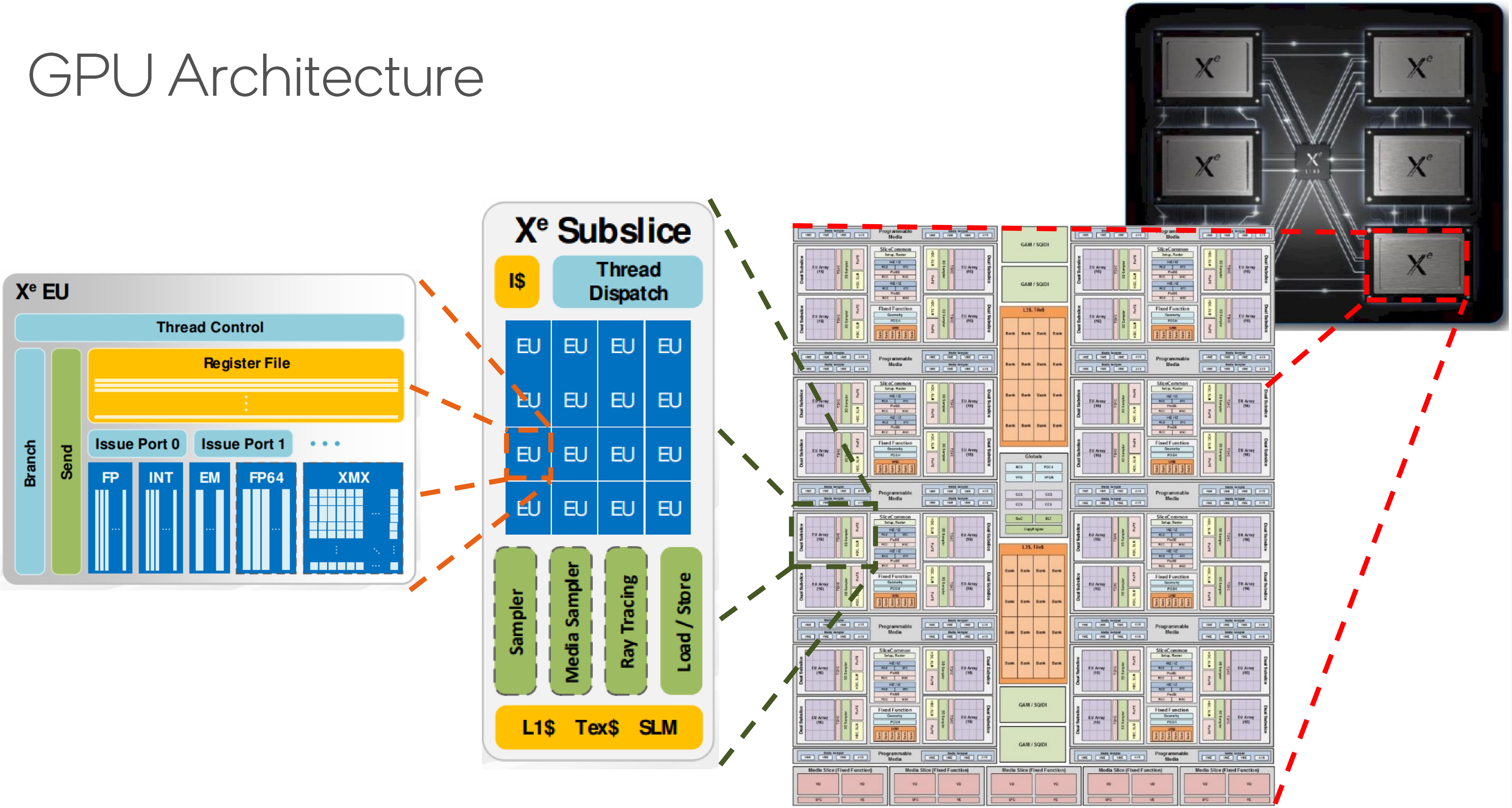
Parallelism

Creating Parallelism on the Target Device

- The `target construct` transfers the control flow to the target device
  - Transfer of control is sequential and synchronous

- OpenMP* separates offload and parallelism
  - Programmers need to explicitly create parallel regions on the target device
  - In theory, this can be combined with any OpenMP construct
  - In practice, there is only a useful subset of OpenMP for a target device (more later)

GPU Architecture



OpenMP* GPU Offload and OpenMP Constructs

- OpenMP GPU offload support all “normal” OpenMP constructs
  - E.g. parallel, for/do, barrier, sections, tasks, etc.
  - Not every construct will be useful

- Full threading model outside of a single GPU subslice not supported
  - No synchronization among subslices
  - No coherence and memory fence between among subslice L1 caches

Example: saxpy

- On the device, the **`parallel`** construct creates a team of threads to be executed on one subslice or stream multiprocessor

```
void saxpy(float a, float* x, float* y,
           int sz) {
#pragma omp target map(to:x[0:sz]) \
                   map(tofrom(y[0:sz])
#pragma omp parallel for simd
    for (int i = 0; i < sz; i++) {
        y[i] = a * x[i] + y[i];
    }
}
```

host

target

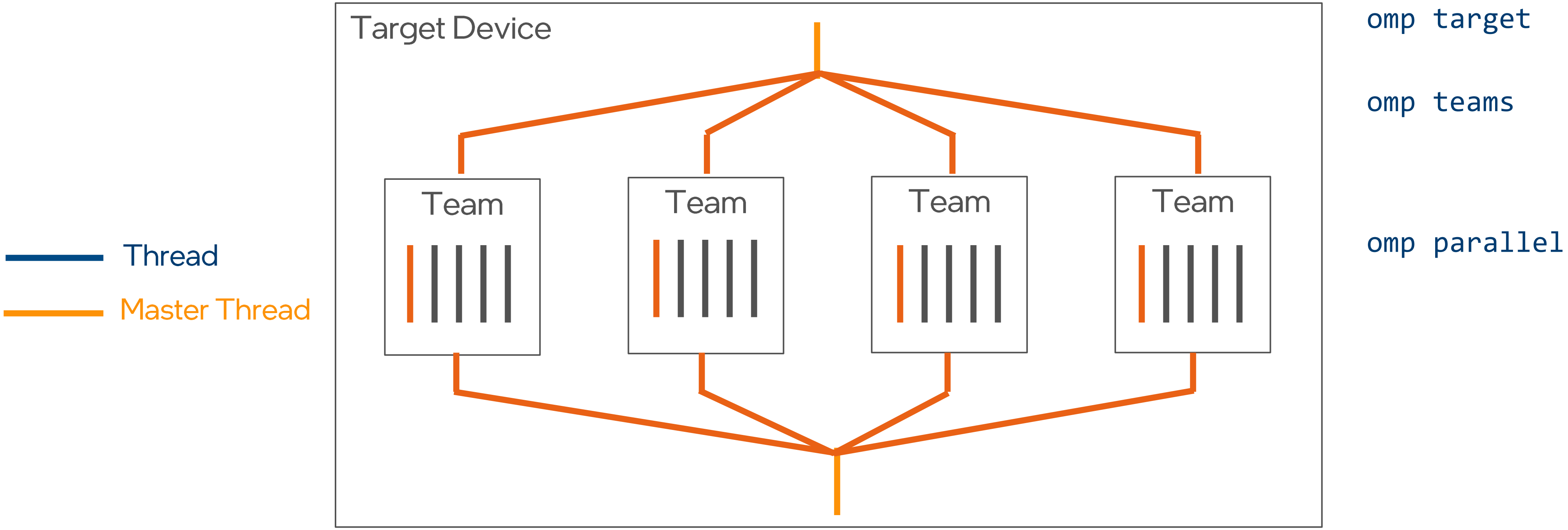
GPUs are multi-level devices: SIMD, threads, thread blocks

Create a team of threads to execute the loop in parallel and SIMDify.
Only one GPU subslice utilized, GPU significantly underutilized

```
icx -fiopenmp -fopenmp-targets=spir64 -o saxpy saxpy.c
```

Teams Construct

- Creates multiple master threads, effectively creates a set of thread teams (league)
- Synchronization does not apply across teams.



`Teams` Construct

- Support multi-level parallel devices
- Syntax (C/C++):

```
#pragma omp teams [clause[[,] clause],…]
structured-block
```

- Syntax (Fortran):

```
!$omp teams [clause[[,] clause],…]
structured-block
```

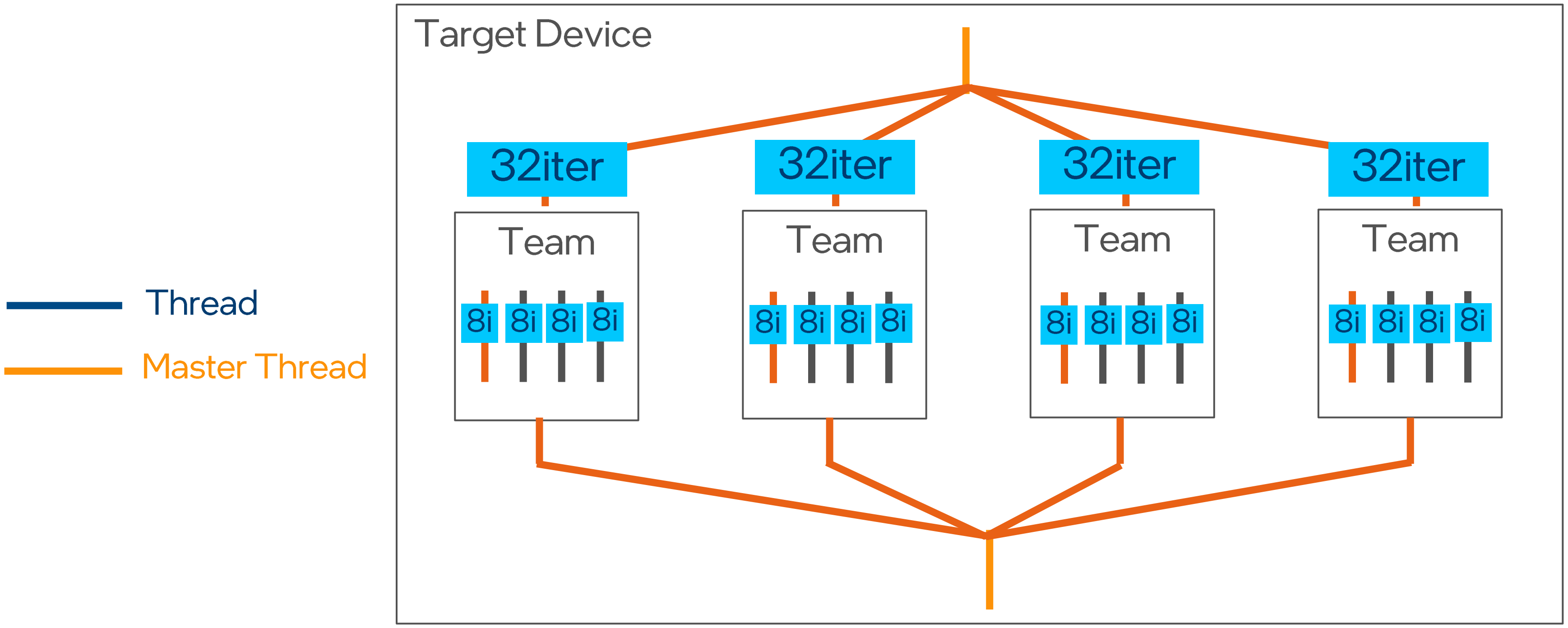
- Clauses

```
num_teams(integer-expression), thread_limit(integer-expression)
default(shared | firstprivate | private none)
private(list), firstprivate(list), shared(list), reduction(operator:list)
```

Distribute Construct

- **`distribute`** construct distributes iterations of a loop across the different teams
  - Worksharing within a league
  - Nested inside a **`teams`** region
  - Can specify distribution schedule
  - Similar to for/do construct for parallel regions
  - Syntax
    - `#pragma omp distribute` *`[clause[[,] clause]…]`*
    - `!$omp distribute` *`[clause[[,] clause]…]`*

Distribute Diagram



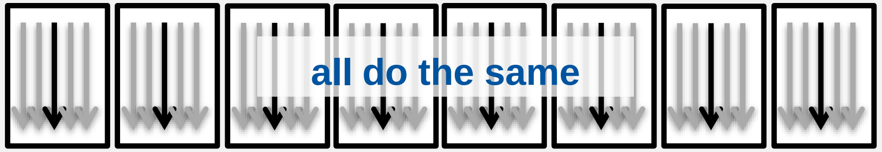

```
omp target

omp teams
omp distribute

omp parallel
omp for/do

omp simd
```

Multi-level Parallel saxpy

```
void saxpy(float a, float* x, float* y, int sz) {
    #pragma omp target map(to:x[0:sz]) map(tofrom(y[0:sz])
    {

        {





            for (ib = 0; ib < sz; ib += num_blocks) {





                for (int i = ib; i < ib + num_blocks; i++) {




                    y[i] = a * x[i] + y[i];
}   }   }   }   }
```

Multi-level Parallel saxpy

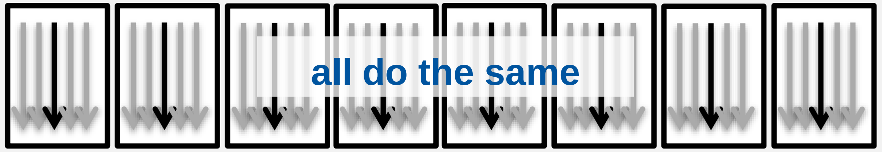
```
void saxpy(float a, float* x, float* y, int sz) {
    #pragma omp target map(to:x[0:sz]) map(tofrom(y[0:sz])
    {
        #pragma omp teams num_teams(num_blocks)
        {
```



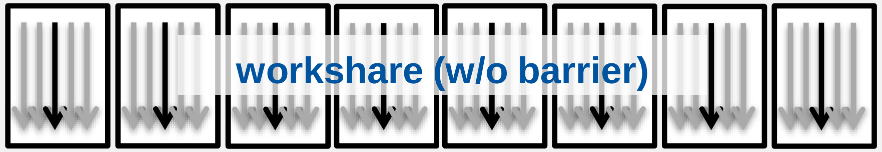

```
            for (ib = 0; ib < sz; ib += num_blocks) {

                for (int i = ib; i < ib + num_blocks; i++) {

                    y[i] = a * x[i] + y[i];
}   }   }   }   }
```

Multi-level Parallel saxpy

```
void saxpy(float a, float* x, float* y, int sz) {
    #pragma omp target map(to:x[0:sz]) map(tofrom(y[0:sz])
    {
        #pragma omp teams num_teams(num_blocks)
        {
```



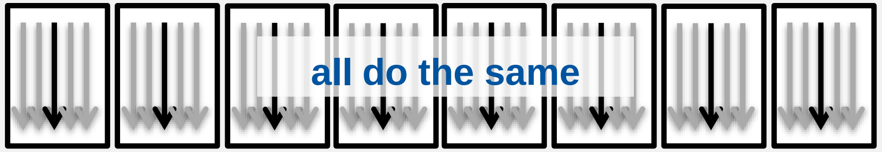

```
            #pragma omp distribute
            for (ib = 0; ib < sz; ib += num_blocks) {
```



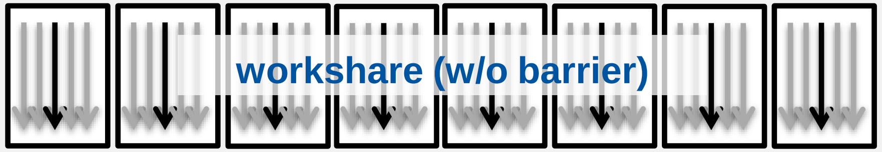

```
                for (int i = ib; i < ib + num_blocks; i++) {



                    y[i] = a * x[i] + y[i];
}   }   }   }   }
```

Multi-level Parallel saxpy

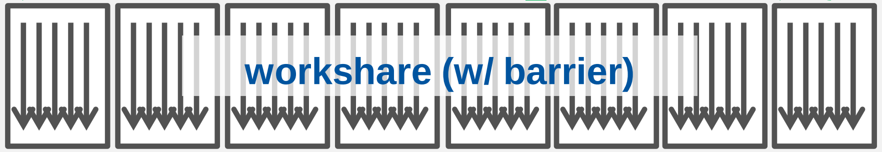
```
void saxpy(float a, float* x, float* y, int sz) {
    #pragma omp target map(to:x[0:sz]) map(tofrom(y[0:sz])
    {
        #pragma omp teams num_teams(num_blocks)
        {
```




```
            #pragma omp distribute
            for (ib = 0; ib < sz; ib += num_blocks) {
```




```
                #pragma omp parallel for simd
                for (int i = ib; i < ib + num_blocks; i++) {
```




```
                    y[i] = a * x[i] + y[i];
}   }   }   }   }
```

Multi-level Parallel saxpy

- For convenience, OpenMP* defines composite construct to implement the required code transformation

```
void saxpy(float a, float* x, float* y, int sz) {
    #pragma omp target teams distribute parallel for simd \
            num_teams(num_blocks) map(to:x[0:sz]) map(tofrom(y[0:sz])
    for (int i = 0; i < sz; i++) {
        y[i] = a * x[i] + y[i];
    }
}
```

```
subroutine saxpy(a, x, y, n)
    ! Declarations omitted
!$omp omp target teams distribute parallel do simd &
!$omp&            num_teams(num_blocks) map(to:x) map(tofrom(y)
    do i=1,n
        y(i) = a * x(i) + y(i)
    end do
!$omp end target teams distribute parallel do simd
end subroutine
```

Complete Saxpy Example

```
void example() {
    float tmp[N], data_in[N], float data_out[N];
#pragma omp target data map(alloc:tmp[:N]) \
                        map(to:a[:N],b[:N]) \
                        map(tofrom:c[:N]) {
        zeros(tmp, N);
        compute_kernel_1(tmp, a); // uses target
        saxpy(2.0f, tmp, b);
        compute_kernel_2(tmp, b); // uses target
        saxpy(2.0f, c, tmp);
}
}
```

```
void zeros(float* a, int n) {
#pragma omp target teams distribute parallel for
    for (int i = 0; i < n; i++)
        a[i] = 0.0f;
}
```

```
void saxpy(float a, float* y, float* x, int n) {
#pragma omp target teams distribute parallel for
    for (int i = 0; i < n; i++)
        y[i] = a * x[i] + y[i];
}
```

Case Study: NWChem TCE CCSD(T)

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NWChem

- Computational chemistry software package
  - Quantum chemistry
  - Molecular dynamics
- Designed for large-scale supercomputers
- Developed at the EMSL at PNNL
  - EMSL: Environmental Molecular Sciences Laboratory
  - PNNL: Pacific Northern National Lab
- URL: http://www.nwchem-sw.org

Finding Offload Candidates

- Requirements for offload candidates
  - Compute-intensive code regions (kernels)
  - Highly parallel
  - Compute scaling stronger than data transfer, e.g., compute $O(n^3)$ vs. data size $O(n^2)$
- Intel® Advisor: Offload Advisor can be used to identify candidates

Example Kernel (1 of 27 in total)

```
      subroutine offl_t_d1_1(h3d,h2d,h1d,p6d,p5d,p4d,
     1                  h7d,triplesx,t2sub,v2sub)
c     Declarations omitted.
      double precision triplesx(h3d*h2d,h1d,p6d,p5d,p4d)
      double precision t2sub(h7d,p4d,p5d,h1d)
      double precision v2sub(h3d*h2d,p6d,h7d)
!$omp target
!$omp teams distribute parallel do private(p4,p5,p6,h2,h3,h1,h7)
      do p4=1,p4d
      do p5=1,p5d
      do p6=1,p6d
      do h1=1,h1d
      do h7=1,h7d
      do h2h3=1,h3d*h2d
       triplesx(h2h3,h1,p6,p5,p4)=triplesx(h2h3,h1,p6,p5,p4)
     1   - t2sub(h7,p4,p5,h1)*v2sub(h2h3,p6,h7)
      end do
      end do
      end do
      end do
      end do
      end do
!$omp end teams distribute parallel do
!$omp end target
      end subroutine
```

1.5GB data transferred (host to device)

1.5GB data transferred (device to host)

- All kernels expose the same structure
- 7 perfectly nested loops
- Some kernels contain inner product loop (then, 6 perfectly nested loops)
- Trip count per loop is equal to "tile size" (20-30 in production)
- Naïve data allocation (tile size 24)
  - Per-array transfer for each `target` construct
  - triplesx: 1458 MB
  - t2sub, v2sub: 2.5 MB

Invoking the Kernels / Data Management

- Simplified pseudo-code

```
!$omp target enter data alloc(triplesx(1:tr_size))
c     for all tiles
      do ...
        call zero_triplesx(triplesx)
        do ...
          call comm_and_sort(t2sub, v2sub)
!$omp target data map(to:t2sub(t2_size)) map(to:v2sub(v2_size))
          if (...)
            call sd_t_d1_1(h3d,h2d,h1d,p6d,p5d,p4d,h7,triplesx,t2sub,v2sub)
          end if
c         same for sd_t_d1_2 until sd_t_d1_9
!$omp target end data
        end do
        do ...
c         Similar structure for sd_t_d2_1 until sd_t_d2_9, incl. target data
        end do
        call sum_energy(energy, triplesx)
      end do
!$omp target exit data release(triplesx(1:size))
```

Allocate 1.5GB data once, stays on device.

Update 4MB of data for (potentially) multiple kernels.

- Reduced data transfers:
  - triplesx:
    - allocated once
    - always kept on the target
  - t2sub, v2sub:
    - allocated after comm.
    - kept for (multiple) kernel invocations

Conclusion

Summary

- OpenMP* offload supported by the Intel® C++ Compiler and Intel® Fortran Compiler as part of the Intel® oneAPI HPC Toolkit
- Use the **`target`** directive to offload
- Use the **`map`** clause with **`target, target data, target enter/exit data`** directives to improve data transfer efficiency
- Use the **`teams/distribute`** directives fully utilize multiple GPU subslices
- Use the **`parallel/for/do`** directive to use the threads within a GPU subslice
- Use the **`simd`** directive for optimal simd execution on GPU execution units

Other Topics of Interest

- Using the Intel® Advisor : Offload Advisor to identify areas of code that are advantageous to offload
  - Provides performance speedup projection on accelerators
- Using the Intel® Advisor: Roofline Analysis to visualize hardware-imposed performance ceilings for the CPU and GPU.
  - Provides insights on bottlenecks and optimization steps

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