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OpenMP Basics

BEAST Lab WS 2022/23

Praktikum Evaluierung moderner HPC-Architekturen und -Beschleuniger



OpenMP

- A method for portable programming of shared memory systems
 - Open specification for Multi-Processing
- **Industry Standard**
 - Guided by the OpenMP Architecture Review Board (ARB)
 - Major companies and research labs participate in the ARB
 - Current version: v5.1 (November 2020)
- Language extension for C/C++ and Fortran
 - Compiler directives
 - Library **routines**
 - Environment variables
- www.openmp.org
 - Current specification, tutorials, other resources



OpenMP Example: Hello World

Source Code:

```
#include <stdio.h>
#include <omp.h>
int main(int argc, char* argv[]) {
#pragma omp parallel
      printf(,,Ahoi OpenMP world\n");
}
```

Compilation:

```
icc -openmp hello.c -o hello
gcc -fopenmp hello.c -o hello
```

The flag to enable OpenMP is implementation-specific

Execution:

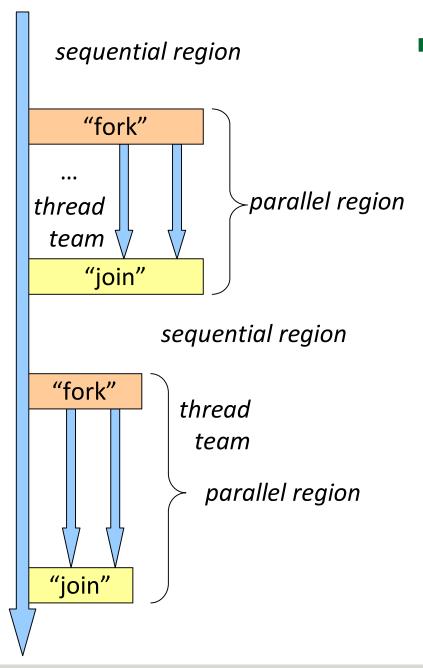
```
>$ export OMP_NUM_THREADS=4
>$ ./hello
Ahoi OpenMP world
Ahoi OpenMP world
Ahoi OpenMP world
Ahoi OpenMP world
```

Execution with 2 threads:

```
>$ export OMP_NUM_THREADS=2
>$ ./hello
Ahoi OpenMP world
Ahoi OpenMP world
```

OpenMP Execution Model

initial thread



- This model is called the **fork-join** Model
 - Program starts with a single thread (called the initial thread)
 - Parallel regions create additional threads (**team threads**), initial thread becomes the master thread in the team
 - Team threads disappear (logically) at the end of a parallel region
 - Implementations may keep team threads around in a thread pool for reasons of efficiency
 - There is an **implicit barrier** at the end of a parallel region
 - Number of threads may change between parallel regions

Creating Threads: #pragma omp parallel

```
#include <stdio.h>
#include <omp.h>
int main(int argc, char* argv[]) {
#pragma omp parallel
    printf(,,Ahoi OpenMP world\n");
}
```

Worksharing constructs are used to distribute work between threads

- for
- sections
- single
- workshare (Fortran only)

The structured block is executed redundantly (in parallel) by all threads

Shared and Private Variables

Variables declared outside the parallel region are shared by default

```
#include <stdio.h>
                            shared by default
#include <omp.h>
double alpha=1.23;
int main(int argc, char* argv[]) {
                               shared by default
   double gamma=23.11;
#pragma omp parallel
                               private by default
        int mydelta;
        #pragma omp for
         for(int i=0; i<100; i++) {
           do_some_work(i, alpha);
                            OK! modifying private copy
      mydelta = ...;
      gamma+=mydelta;
```

- Shared variables
 - Are accessible by all threads (only one copy exists)
- Private variables
 - Accessible only by one thread (each thread has its own copy)
- Data sharing clauses can override defaults

!!!Warning: modifying shared variable!!! Needs some form of synchronization, e.g., atomic, critical, locks

Data Sharing Clauses (Parallel and Work Sharing Constructs)

- private(var-list)
 - Variables in var-list are private
- shared(var-list)
 - Variables in var-list are shared
- **default**(private | shared | none)
 - Sets the default for all variables in this region
 - Default none raises compiler error if sharing is not explicitly specified
- firstprivate(var-list)
 - Variables are private and are initialized with the value of the shared copy before the region
- lastprivate(var-list)
 - Variables are private and the value of the thread executing the last iteration of a parallel loop in sequential order is copied to the variable outside of the region.

Initialization of Private Variables

```
int i, j;
i = 1;
j = 2;
#pragma omp parallel private(i) firstprivate(j)
  printf(,,i=%d j=%d\n", i, j);
```

Execution:

```
>$ export OMP_NUM_THREADS=4
>$ ./a.out
i=5456498 j=2
i = -732837541 j = 2
i=788564 j=2
i=821656 j=2
```

- Private copies of i are not initialized!
- Firstprivate copies of j are initialized to the outside value

Worksharing in Parallel Regions

Goal: distribute work among threads in a parallel region

```
#include <stdio.h>
#include <omp.h>
int main(int argc, char* argv[]) {
  int i;
#pragma omp parallel
        #pragma omp for
        for(i=0; i<100; i++) {
          do_some_work(i);
```

```
// shorthand notation for the above
// combined parallel-workshare
#pragma omp parallel for
```

The omp for construct

- Specifies that the work (loop iterations) should be distributed to the available threads
- Asserts that the loop iterations are independent and can be parallelized

Parallel Loop (C/C++)

```
#pragma omp for [clause[[,] clause]
   for(i=0; i<..; i++..) { .. }
```

- Loop iterations are distributed between the threads of the team
 - A loop scheduling clause specifies exactly how
 - Loop scheduling options: static, dynamic, guided, auto, and runtime
 - E.g., schedule(static)

Characteristics:

- The is no synchronization (i.e., barrier) at the entry of the loop
- There is an implicit barrier at the end of the loop unless a nowait clause is specified
- The loop iteration variable is private by default
- Only simple (so-called canonical forms) of loops are supported
 - Integer iteration variable, only modified in the increment expression
 - Iteration count can be computed before executing the loop

Loop Scheduling Strategies

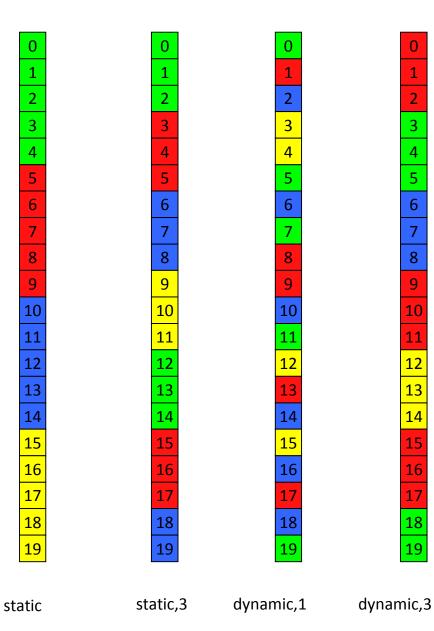
#pragma omp for schedule(type[, size])

- Scheduling type is one of:
 - static: chunks of iterations of the specified size are distributed among threads in a round-robin fashion
 - dynamic: Threads request chunks of the specified size from the runtime;
 when finished executing, a thread requests a new chunk
 - guided: like dynamic, but the chunk size is proportional to remaining work;
 size parameter specifies the minimal chunk size
 - auto: decision is delegated to the compiler and/or runtime system
 - runtime: defer scheduling decision to runtime selection (via environment variable OMP_SCHEDULE); note that it is only possible to specify one schedule for all loops via an environment variable

Loop Scheduling Example

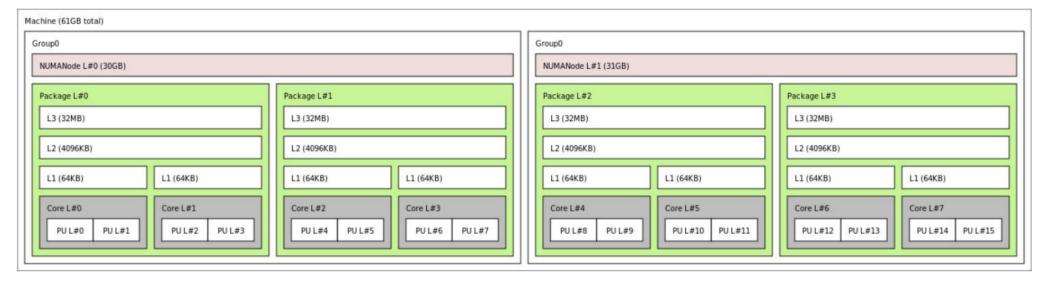
```
#pragma omp parallel
//#pragma omp for schedule(static)
//#pragma omp for schedule(static,3)
//#pragma omp for schedule(dynamic,1)
#pragma omp for schedule(dynamic,3)
       for(i=0; i<20; i++) {
         do_some_work(i);
  }
```

- Thread 0
- Thread 1
- Thread 2
- Thread 3



Thread Affinity

- How threads are mapped to hardware may influence performance
 - E.g., placement of threads to optimize cache sharing vs. memory bandwidth
 - HWLoc output example



- OpenMP allows the specification of
 - What we consider the unit of locality
 OMP_PLACES env. variable = threads | cores | sockets
 - How to distribute threads to places
 - OMP_PROC_BIND env. variable and proc_bind clause
 master | spread | close

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OMP PLACES Env. Variable

- **OMP_PLACES** specifies a list of places where threads should be executed
 - sockets each place corresponds to a single socket, a socket can have multiple cores
 - cores each place corresponds to a single core, each core can have multiple hardware threads
 - threads each place corresponds to a single hardware thread

export OMP_PLACES=cores

- Places and place lists can also be specified numerically
 - Meaning of numeric IDs depends on the system (/proc/cpuinfo, lscpu)

export OMP_PLACES={0,1,2,3}, {4,5,6,7}, ...

OMP_PROC_BIND Env. Variable and proc_bind clause

- OMP_PROC_BIND(policy) or proc_bind(policy) clause specify how threads are mapped onto places
 - master each thread in the team is assigned to the same place as the master thread
 - close threads in the team are placed close to the master thread
 - spread threads are spread evenly over the places

Examples (HW as in Hwloc example)

Parallel region with two threads, one per socket

OMP_PLACES=sockets

#pragma omp parallel num_threads(2) proc_bind(spread)

Parallel region with four threads, all on one socket

OMP_PLACES=cores

#pragma omp parallel num_threads(4) proc_bind(close)

Optimizing for NUMA (1)

NUMA=Non-Uniform-Memory Access

- Accessing local data is beneficial for performance
- Virtual memory is mapped to physical memory in the granularity of pages (typically 4KB)
- Usually where a memory page gets allocated is determined by a first touch **policy** (i.e., local to the core that first uses a memory page)
- This implies that the initialization of data structures should reflect the intended later access patterns
- Bad: Serial initialization and parallel access
- Bad: Different parallel initialization and parallel access
- Good: Parallel initialization and parallel access in same way

Other options:

Explicit control using OS mechanisms, e.g., numactl

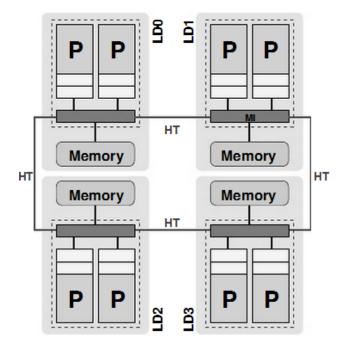
Optimizing for NUMA (2)

Bad: serialized initialization leads to allocation of B,C,D all in one locality domain

```
// initialize data strucutres
for(i=0; i<N; i++ ) {
  B[i]= . . .
 C[i]= . . .
 D[i]= . . .
#pragma omp parallel for
for( i=0; i<N; i++ ) {
 A[i] = B[i] + C[i] * D[i];
```

Good: parallel initialization in the same way it is later accessed (distributed across locality domains)

```
// initialize data strucutres in parallel
#pragma omp parallel for
for(i=0; i<N; i++ ) {
  B[i]= . . .
 C[i]= . . .
 D[i]= . . .
#pragma omp parallel for
for( i=0; i<N; i++ ) {
  A[i] = B[i] + C[i] * D[i];
```



ccNUMA system with four locality domains

> Image source: Hager, Wellein: "Introduction to High Performance Computing for Scientists and Engineers"