Introdução à Programação Multithreaded: explorando arquiteturas heterogêneas e vetorização com OpenMP 4.0

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Agenda

- NCC Presentation
- Parallel architectures
- OpenMP
- Vectorization
- Offload
- Thread league
- N-body

Material

- **Source-code, Slides and Book Chapter:**

- https://github.com/intel-unesp-mcp/talks-source-code/tree/master/OpenMP4

UNESP Center for Scientific Computing

- Consolidates scientific computing resources for São Paulo State University (UNESP) researchers
  - It mainly uses Grid computing paradigm
- Users
  - UNESP researchers, students, and software developers
  - SPRACE project (São Paulo Research and Analysis Center)
    - Caltech, Fermilab, CERN
    - São Paulo CMS Tier-2 Facility

UNESP Center for Scientific Computing

SPRACE - CMS Tier2 Facility

- 144 worker nodes
  - Physical/Logical CPUs: 288/1088
  - HEPSpec06: 13698
- 02 head nodes
- 04 auxiliary servers
- 12 storage servers
  - 1 PB (raw), 0.85 PB (effective): 81% usage
- CSC Network
  - LAN: 1 Gbps & 10 Gbps
  - MAN: 10 Gbps & 100 Gbps
  - WAN: 4x10Gbps & 100 Gbps

Intel ® Partnership

- IPCC (Intel Parallel Computing Center)
  - Vectorization of Geant (**GE**ometry **AN**d **T**racking)
- Intel Modern Code
  - Workshops and Tutorials
    - ❑ High Performance Computing (HPC)
    - ❑ Big Data
  - HPC Consultancy
  - http://modern-code.ncc.unesp.br/

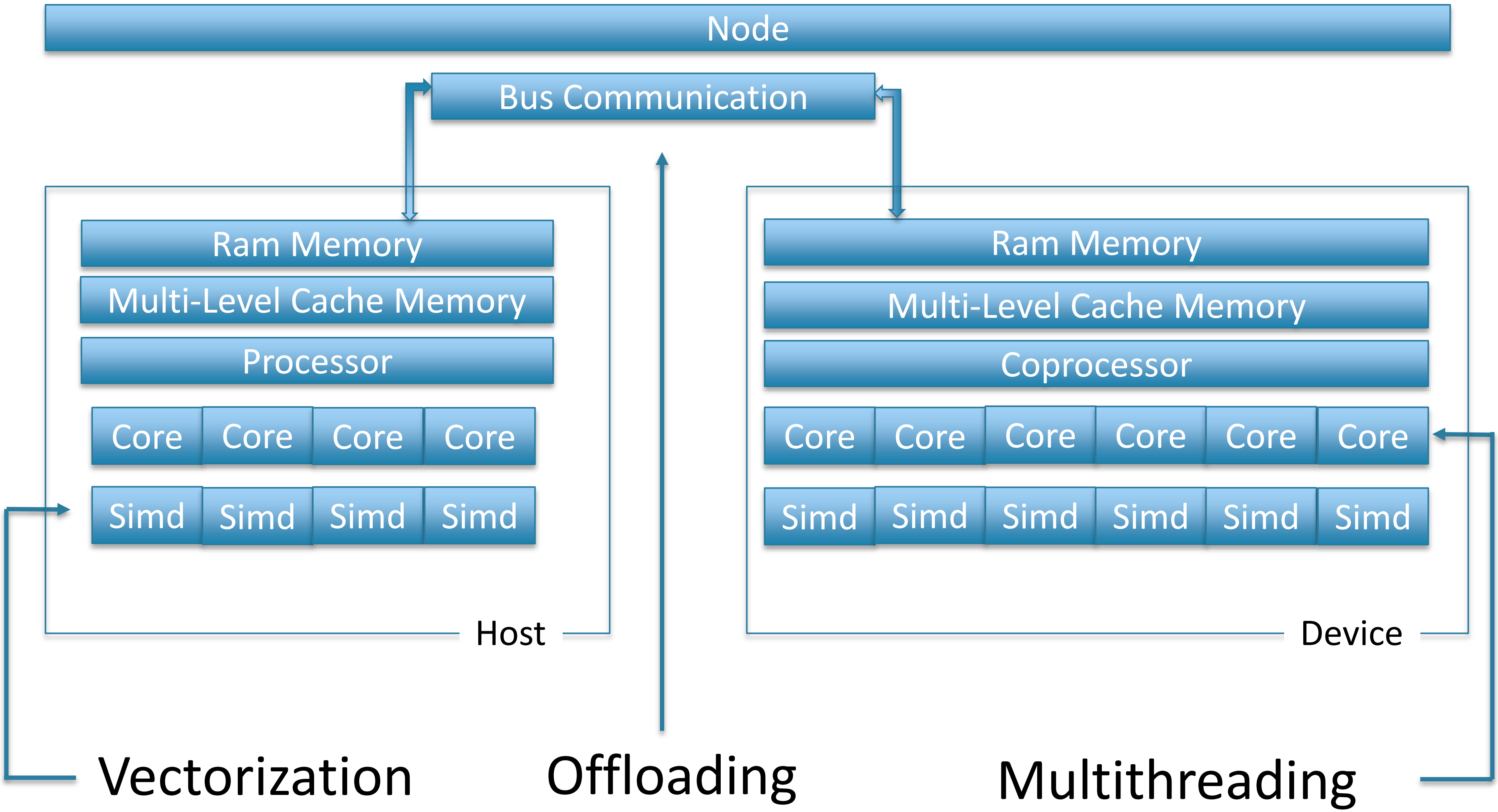
Agenda

- NCC Presentation 5 min
- Parallel architectures 12 min
- OpenMP 15 min
- Vectorization 25 min
- Offload 25 min
- Thread league 20 min
- N-body 20 min

Parallel Architectures

- Heterogeneous computational systems:
  - Multicore processors;
  - Multi-level memory sub-system;
  - Input and Output sub-system;
- Multi-level parallelism:
  - Processing core;
  - Chip multiprocessor;
  - Computing node;
  - Computing cluster;
- Hybrid Parallel architectures
  - Coprocessors and accelerators;

Hybrid Parallel Architectures



Hybrid Parallel Architectures

- Exploring parallelism in hybrid parallel architectures
  - Multithreading
  - Vectorization
    - ❑ Auto vectorization;
    - ❑ Semi-auto vectorization;
    - ❑ Explicit vectorization;
  - Offloading
    - ❑ Offloading code to device;
- OpenMP 4.0;
  - Supports vectorization and offloading on hybrid parallel architectures;

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- Hybrid Parallel Architectures
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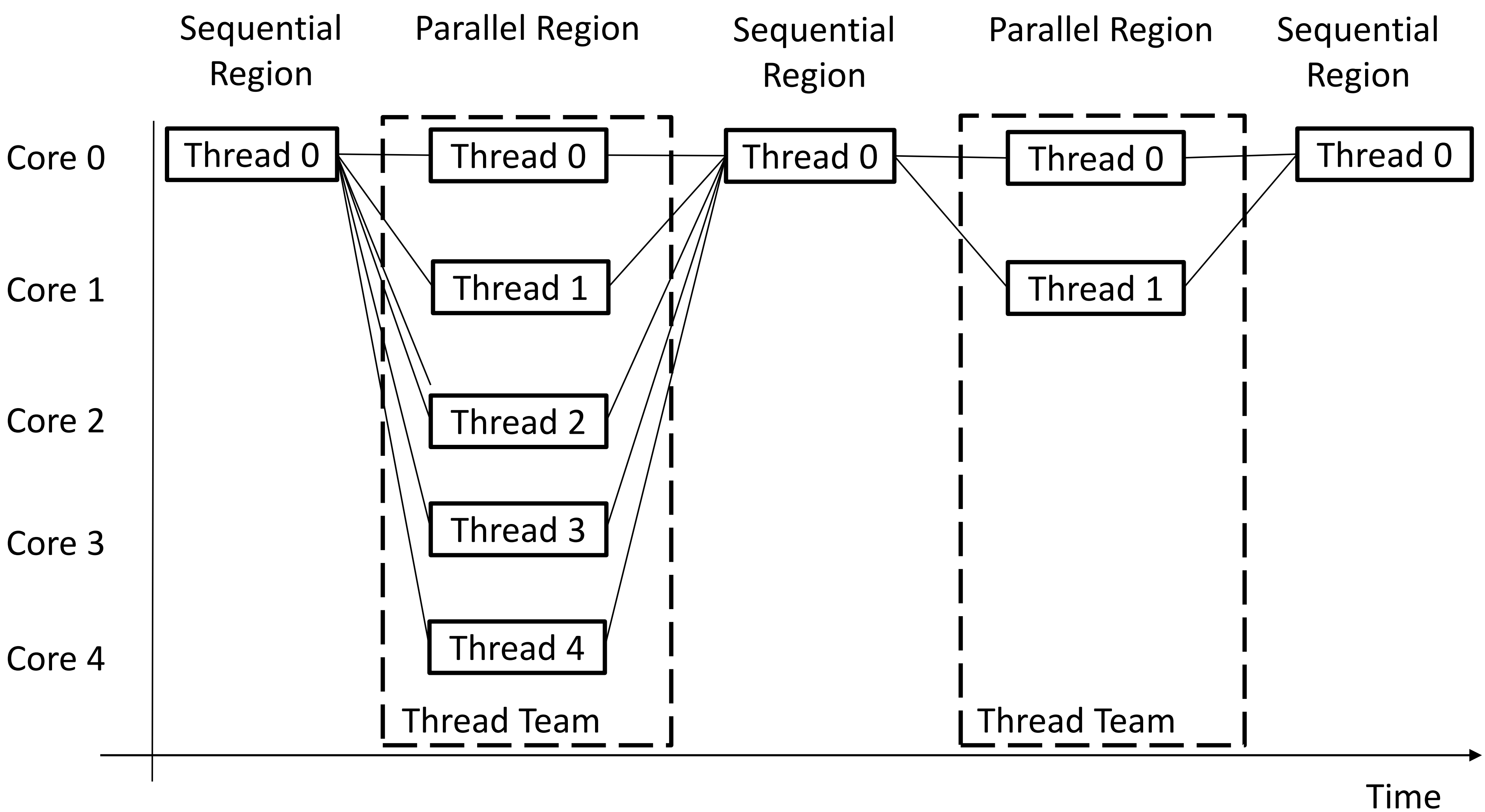
OpenMP

- OpenMP is an acronym for Open Multi-Processing
- An Application Programming Interface (API) for developing parallel programs in shared memory architectures
- Three primary components of the API are:
  - Compiler Directives
  - Runtime Library Routines
  - Environment Variables
- de facto standard -- specified for C, C++, and FORTRAN
- http://www.openmp.org/
  - specification, examples, tutorials and documentation

OpenMP



Sequential Region
Parallel Region
Sequential Region
Parallel Region
Sequential Region
Core 0
Core 1
Core 2
Core 3
Core 4
Thread 0
Thread 0
Thread 1
Thread 2
Thread 3
Thread 4
Thread 0
Thread 0
Thread 1
Thread 0
Thread Team
Thread Team
Time

OpenMP: the core elements

Parallel control structures

- Form a team of threads and execute them in parallel
- `omp parallel`

Work sharing

- Distribute work among threads
- ```
  omp [parallel] loop
  omp [parallel] sections
  omp [parallel] workshare
  omp single
  ```

Data environment

- Control variables scope
- `omp threadprivate`
  `shared/*private` clauses

Synchronization

- Coordinates thread execution
- ```
  omp atomic
  omp barrier
  omp critical
  omp flush
  omp master
  omp ordered
  omp taskgroup
  omp taskwait
  ```

OpenMP 4.0

SIMD vectorization

- Control execution on hardware supporting SIMD instructions
- ```
  omp simd
  omp declare simd
  omp [parallel] loop simd
  ```

Offload execution

- Control execution on coprocessor devices
- ```
  omp declare target
  omp distribute
  omp target [data|update]
  omp teams
  ```

Tasking

- Structures for deferring execution
- ```
  omp task
  omp taskyield
  ```

Runtime environment

- Runtime functions and environment variables
- `omp_set_num_theads()`, etc.
  `OMP_SCHEDULE`, etc.
  ```

OpenMP parallel processing model

```
main() {
    …
    #pragma omp parallel {
        #pragma omp sections {
            #pragma omp section
            { … }
            #pragma omp section
            { … }
        }
        …
        #pragma omp for nowait
        for( … ) {
            …
        }
        #pragma omp critical
        { … }
        …
        #pragma omp barrier
        …
    }
    …
}
```

Begin serial execution. Only the initial thread executes.

Begin a parallel construct and form a team.

Begin a worksharing construct with two units of work.

Wait until both units of work complete.

Begin a “non-blocking” worksharing construct.
Each iteration chunk is unit of work.
Work is distributed among the team members.

This code is executed by each team member.

Critical section.
Only one thread executes at a time.

End of worksharing construct. “nowait” was specified so threads proceed.

Wait for all team members to arrive.

This code is executed by each team member.

End of Parallel Construct
Disband team and continue serial execution.
Possibly more parallel constructs after.

End serial execution.

OpenMP Sample Program

```
N=25;
#pragma omp parallel for
for (i=0; i<N; i++)
    a[i] = a[i] + b;
```

	Thread 0					Thread 1					Thread 2					Thread 3					Thread 4				
i=	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24

OpenMP Sample Program

```
#include <stdio.h>
#include <stdlib.h>
#include <omp.h>
#include <unistd.h>

int main() {
  int thid; char hn[600], i;
  double res, p[100];

  #pragma omp parallel
  {
    gethostname(hn,600);
    printf("hostname %s\n",hn);
  }
  res = 0;

  #pragma omp for
  for ( i = 0 ; i < 100 ; i++ ) {
    p[i] = i/0.855;
  }

  #pragma omp for
  for ( i = 0 ; i < 100 ; i++ ) {
    res = res + p[i];
  }

  printf("sum: %f", res);
}
```

Compiling and running an OpenMP Application

#Build the application for Multicore Architecture (Xeon)

icc *<source-code>* -o *<omp_binary>* -fopenmp

#Build the application for the ManyCore Architecture (Xeon Phi)

icc *<source-code>* -o *<omp_binary>*.mic -fopenmp -mmic

#Launch the application on host

./*omp_binary*

#Launch the application on the device from host

micnativeloadex ./*omp_binary.mic* -e "LD_LIBRARY_PATH=/opt/intel/lib/mic/"

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- N-body

Intel Advisor

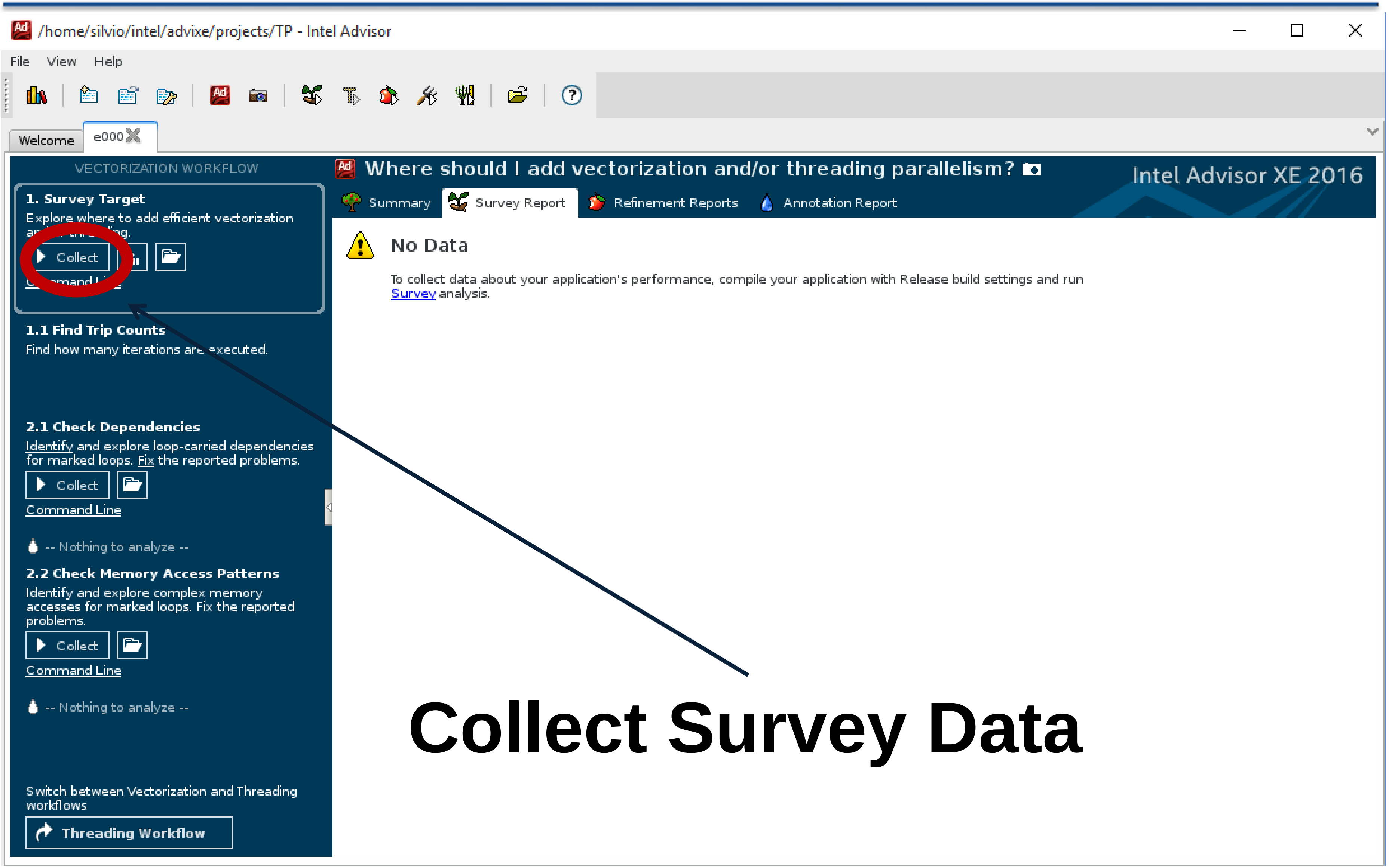
- Evaluate multi-threading parallelization

- Intel® Advisor XE
  - ❑ Performance modeling using several frameworks for multi-threading in processors and co-processors:
    - OpenMP, Intel® Cilk ™ Plus, Intel® Threading Bulding Blocks
    - C, C++, Fortran (OpenMP only) e C# (Microsoft TPL)
  - ❑ Identify parallel opportunities
  - ❑ Scalability prediction: amount of threads/performance gains
  - ❑ Correctness (deadlocks, race condition)

Intel Advisor

- Intel Advisor Analysis:
  - Survey
    - Vectorization of loops: detailed information about vectorization;
    - Total Time: elapsed time on each loop considering the time involved in internal loops;
    - Self Time: elapsed time on each loop disconsidering the time involved in internal loops;
  - Suitability
    - Speedup gains that may be obtained parallelizing annotated loops;

Intel Advisor - Survey Data



Collect Survey Data

Vectorization

- Instructs the compiler to enforce vectorization of loops (**Semi-auto vectorization**)

- omp simd
  - marks a loop to be vectorized by the compiler
- omp declare simd
  - marks a function that can be called from a SIMD loop to be vectorized by the compiler
- omp parallel for simd
  - marks a loop for thread work-sharing as well as SIMDing

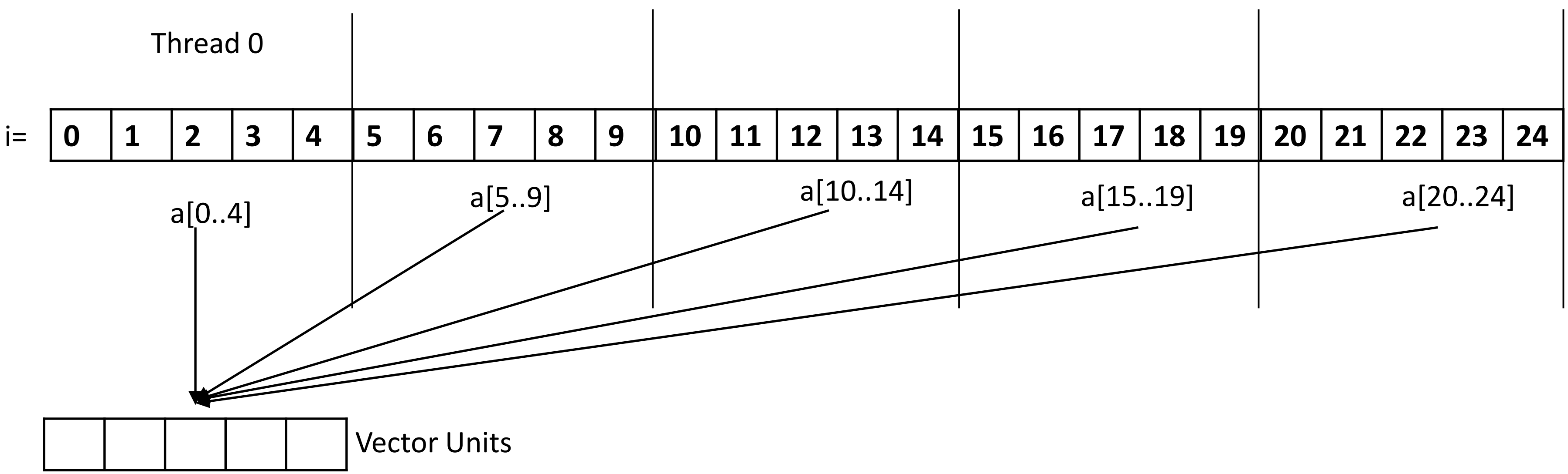
OMP SIMD

- Vectorize a loop nest
  - Cut loop into chunks that fit a SIMD vector register
  - No parallelization of the loop body

- Syntax

```
#pragma omp simd [clause[[,] clause],…]
for-loops
```

```
N=25;
#pragma omp simd
for (i=0; i<N; i++)
   a[i] = a[i] + b;
```



Data Sharing Clauses

- Specifies that each thread has its own instance of a variable:
  - private(*var-list*): uninitialized vectors for variables in *var-list*
  - firstprivate(*var-list*): Initialized vectors for variables in *var-list*
  - lastprivate(*var-list*):
    - similar to private clause
    - Private copy of last iteration is copied to the original variable
  - reduction(*op*:*var-list*): create private variables for *var-list* and apply reduction operator *op* at the end of the construct

SIMD Loop Clauses

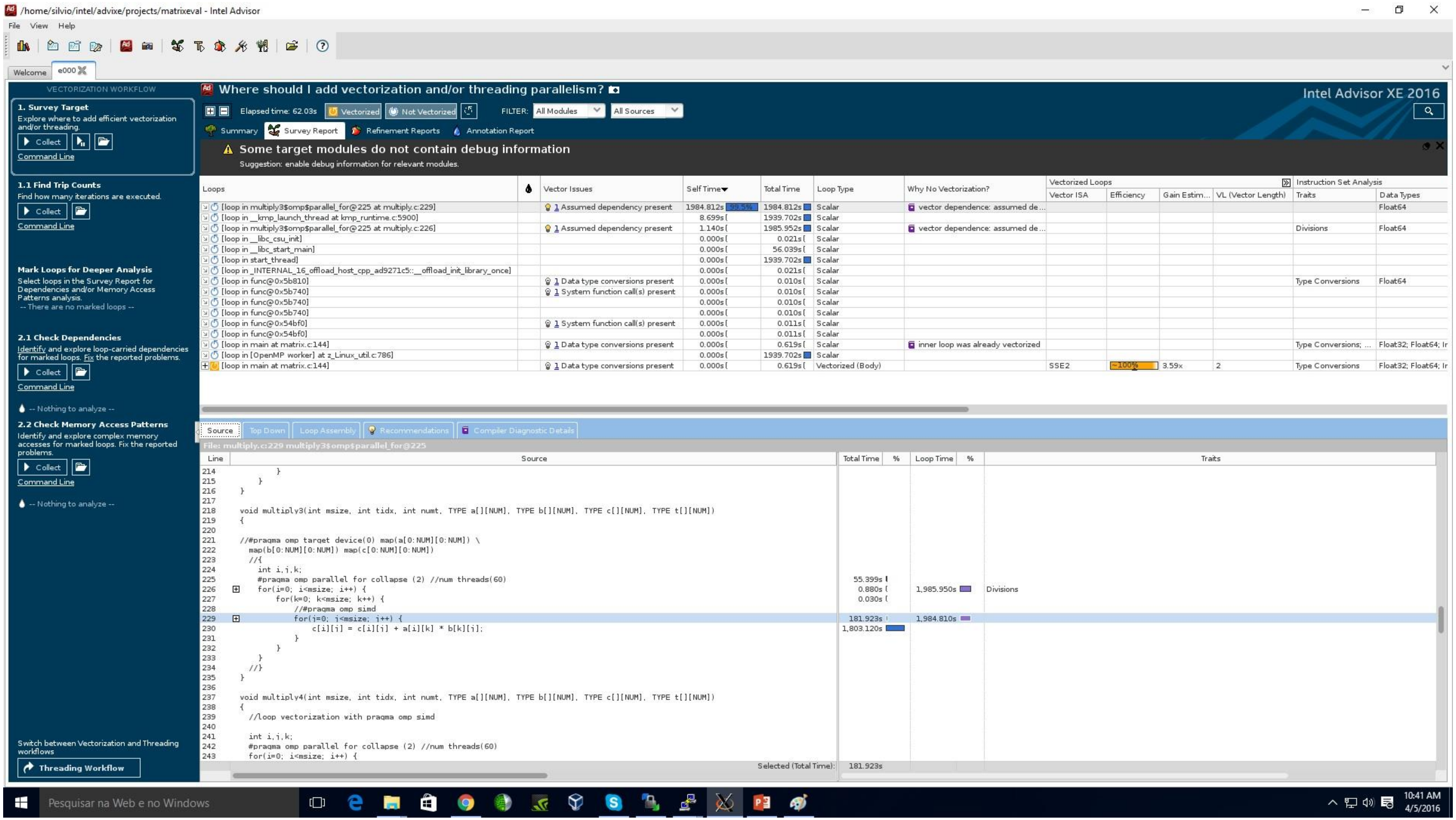
- safelen (*length*)
  - Maximum number of iterations that can run concurrently without breaking a dependence
- linear (*list*[:*linear-step*])
  - The variable's value is in relationship with the iteration number

    $x_i = x_{orig} + i * \text{linear-step}$
- aligned (*list*[:*alignment*])
  - Specifies that the list items have a given alignment
  - Default is alignment for the architecture
- collapse (*n*)
  - Groups two or more loops into a single loop

Pragma OMP simd Example

```
#pragma omp parallel for colapse (2)
for ( i=0; i <msize ; i ++) {
    for ( k=0; k<msize ; k++) {
        #pragma omp simd
        for ( j=0; j<msize ; j++) {
            c[i][j] = c[i][j] + a[i][k] * b[k][j] ;
        }
    }
}
```

OMP SIMD – vectorization Report



SIMD Function Vectorization

- Declare one or more functions to be compiled for calls from a SIMD-parallel loop

- Syntax (C/C++):

```
#pragma omp declare simd [clause[[,] clause],…]
[#pragma omp declare simd [clause[[,] clause],…]]
[…]
function-definition-or-declaration
```

SIMD Function Vectorization

- simdlen (*length*)
  - generate function to support a given vector length
- uniform (*argument-list*)
  - argument has a constant value between the iterations of a given loop
- inbranch
  - function always called from inside an if statement
- notinbranch
  - function never called from inside an if statement

- linear (*argument-list[:linear-step]*)
- aligned (*argument-list[:alignment]*)
- reduction (*operator*:list)

pragma OMP declare simd

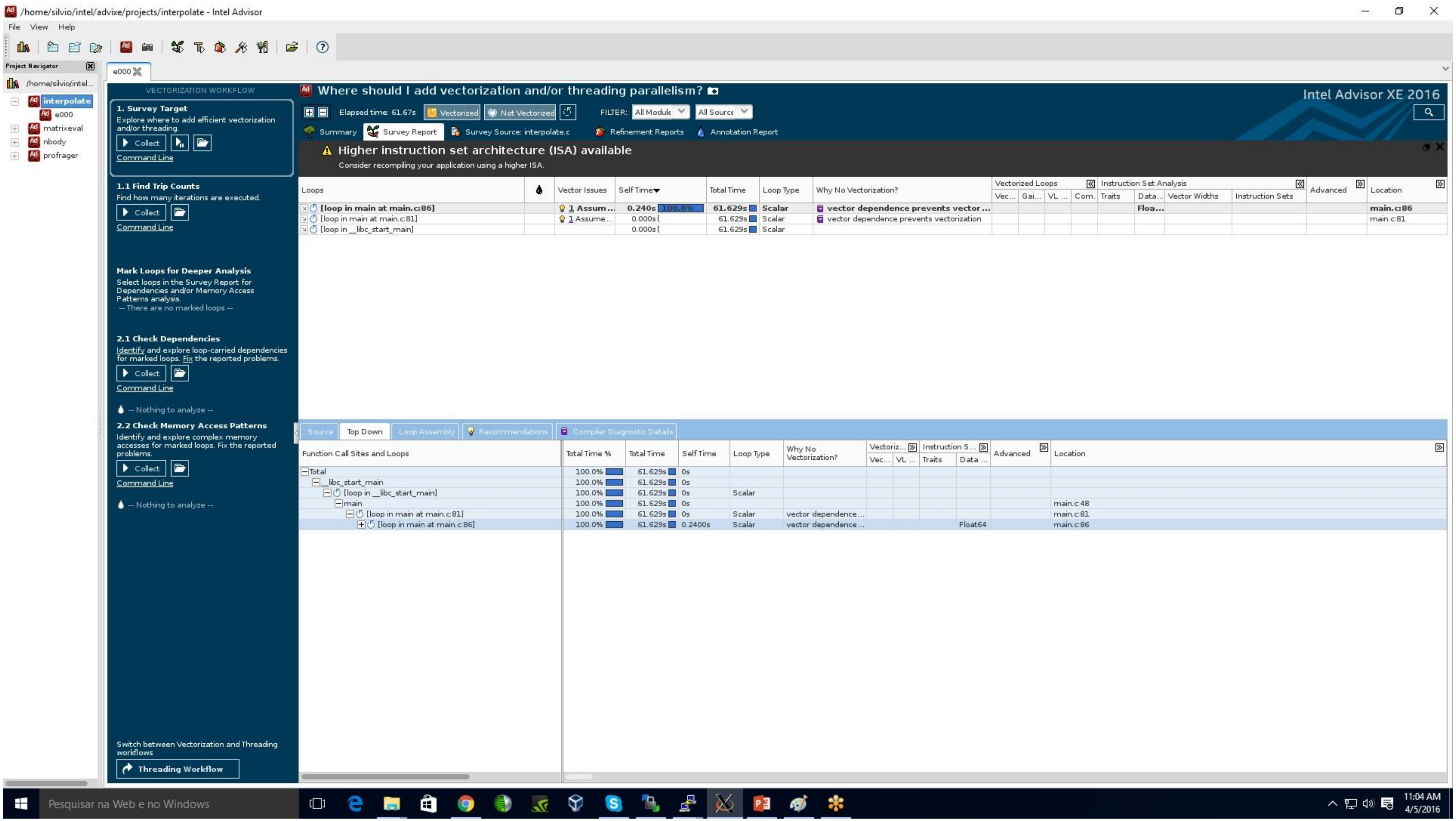
```
#pragma omp declare simdlen (SIMD_LEN)
int FindPosition(double x) {
   return (int)(log(exp(x*steps)));
}

#pragma omp declare simd uniform (vals)
double Interpolate(double x, const point*
vals)
{
   int ind = FindPosition(x);
   ...

   return res;
}
```

```
int main ( int argc , char argv [] )
{
   . . .
   #pragma omp simd
   for ( i=0; i <ARRAY_SIZE;++ i ) {
      dst[i] = Interpolate( src[i], vals ) ;
   }
   . . .
}
```

OMP Declare Simd Vectorization Report



pragma OMP for simd

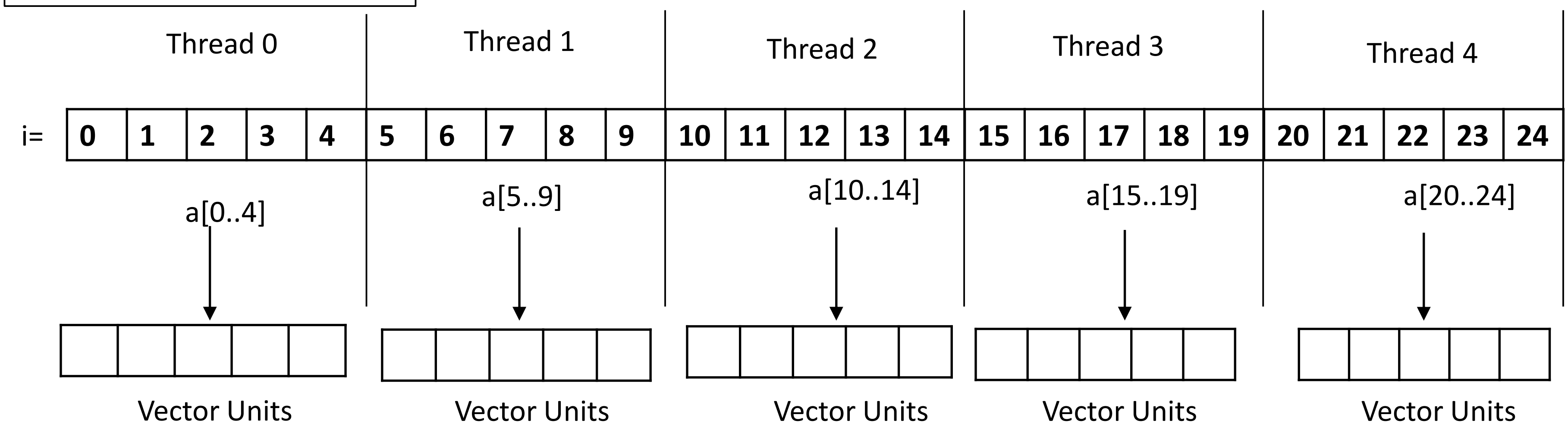
- Parallelize and vectorize a loop nest
  - Distribute a loop's iteration space across a thread team
  - Subdivide loop chunks to fit a SIMD vector register

- Syntax

  `#pragma omp for simd` *`[clause[[,] clause],…]`*

  `for-loops`

```
N=25;
#pragma omp for simd
for (i=0; i<N; i++)
  a[i] = a[i] + b;
```



pragma OMP for simd

```
#pragma omp parallel for simd
for(i=0; i<msize; i++) {
    a[i][j] = distsq(a[i][j], b[i][j])-auxrand;
    b[i][j] += min(a[i][j], b[i][j])+auxrand;
    c[i][j] = (min(distsq(a[i][j], b[i][j]), a[i][j]))/auxrand;
}
```

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OpenMP 4.0 Offload

- **target:** transfers the control flow to the target device
  - Transfer is sequential and synchronous
  - Transfer clauses control data flow
- **target data:** creates a scoped device data environment
  - Does not include a transfer of control
  - Transfer clauses control data flow
  - The device data environment is valid through the lifetime of the target data region
- **target update:** request data transfers from within a target data region
- **omp declare target:** creates a structured-block of functions that can be offloaded.

OpenMP 4.0 Offload Report

- OFFLOAD REPORT:
  - Measures the amount of time it takes to execute an offload region of code;
  - Measures the amount of data transferred during the execution of the offload region;
  - Turn on the report: Export OFFLOAD_REPORT=2

- **[Var]** The name of a variable transferred and the direction(s) of transfer.
- **[CPU Time]** The total time measured for that offload directive on the host.
- **[MIC Time]** The total time measured for executing the offload on the target.
- **[CPU->MIC Data]** The number of bytes of data transferred from the host to the target.
- **[MIC->CPU Data]** The number of bytes of data transferred from the target to the host.

pragma OMP target

- Transfer control [and data] from the host to the device

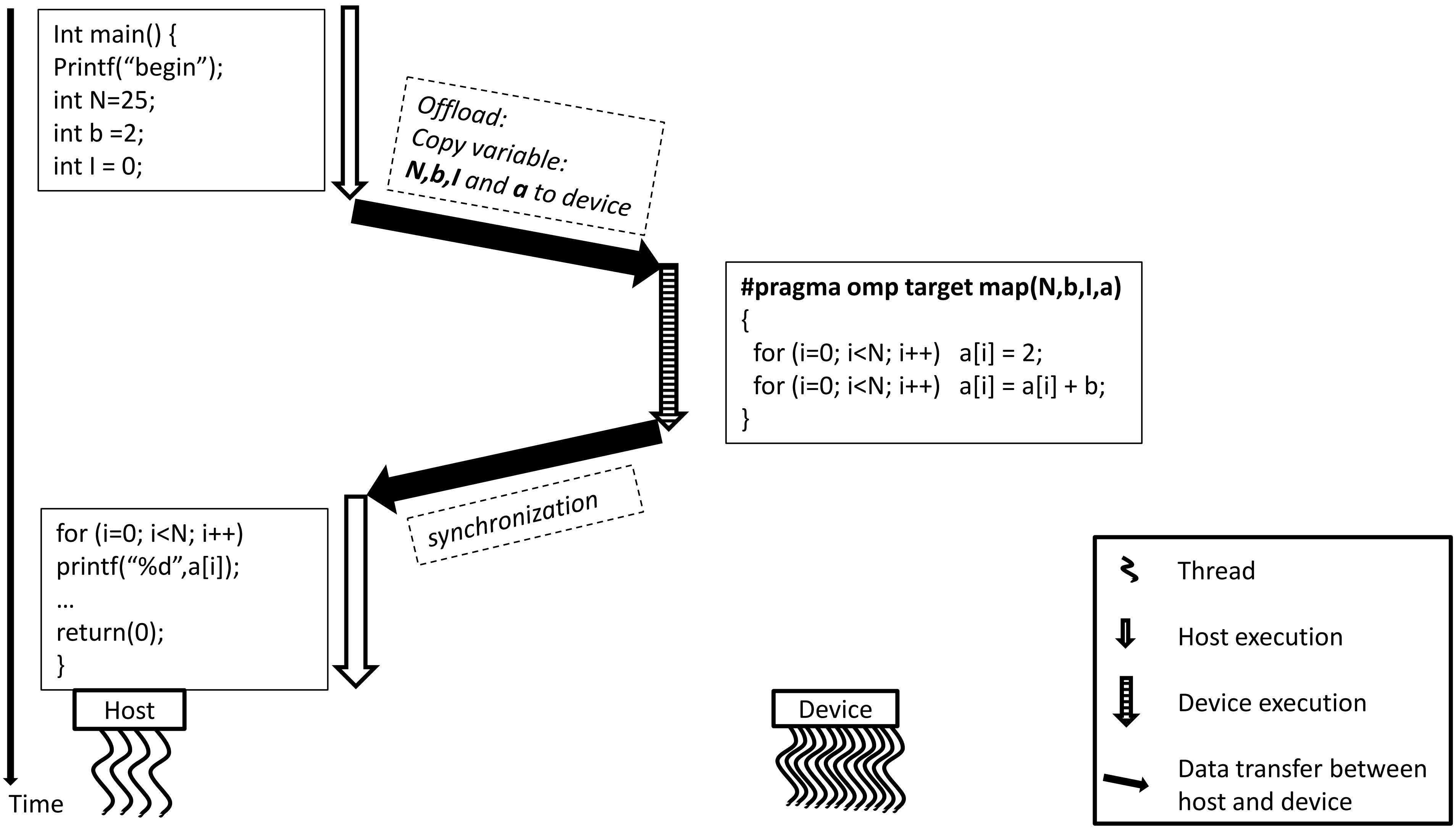
- Syntax
  - `#pragma omp target [data]` *[clause[[,] clause],…]*
    structured-block

- Clauses
  - device(*scalar-integer-expression*):
    - device to offload code;
  - map(alloc | to | from | tofrom: *list*) :
    - map variables to device;
  - if(*scalar-expr*) :
    - test an expression before offload:
      - True executes on device;
      - False executes on host;

pragma OMP target

- Map clauses:
  - alloc : allocate memory on device;
  - to : transfer a variable from host to device;
  - from : transfer a variable from device to host;
  - tofrom :
    - transfer a variable from host to device before start execution;
    - transfer a variable from device to host after finish execution;

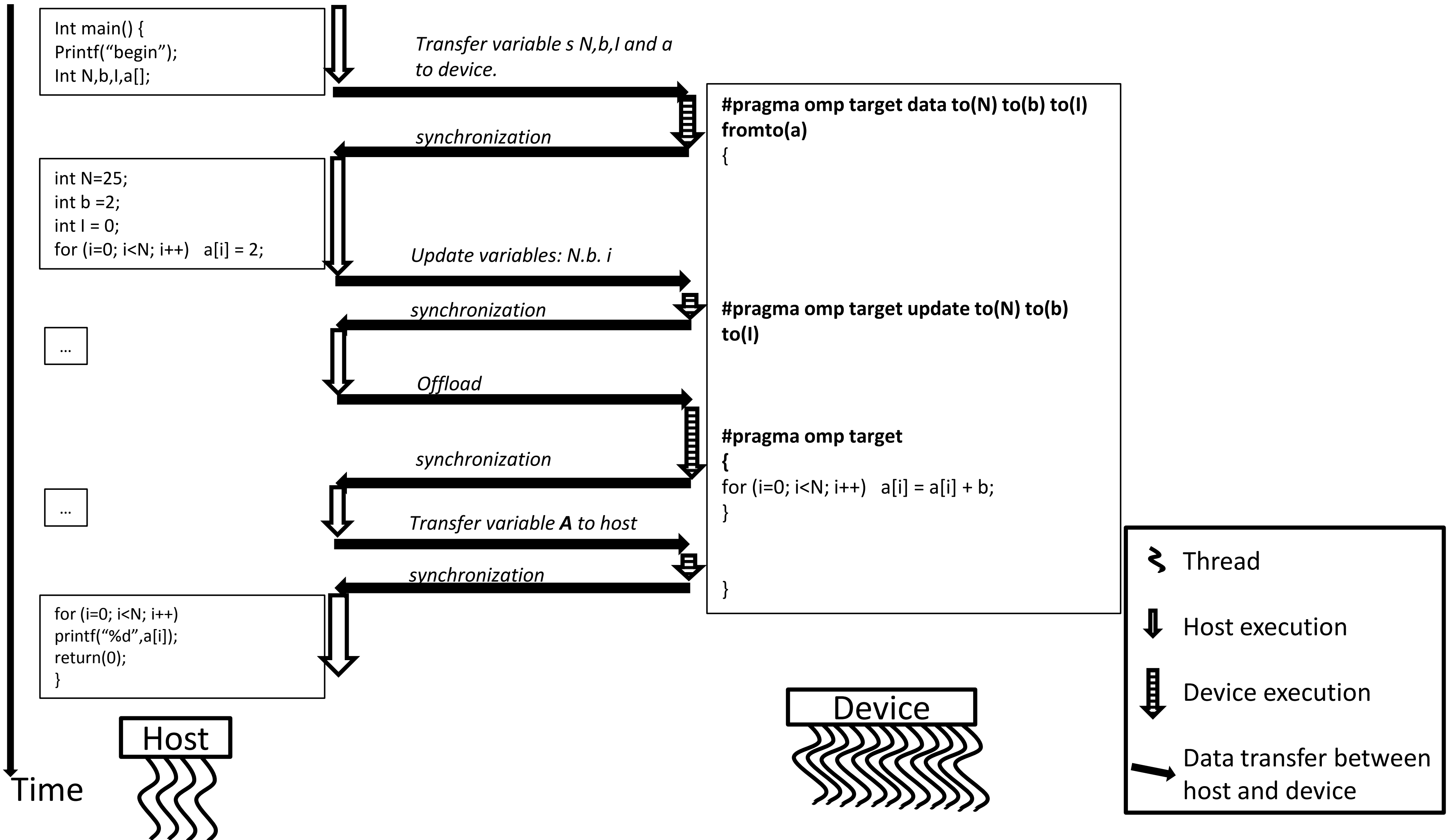
Offloading – OMP Target



pragma OMP target

```
#pragma omp target device(0) map(a[0:NUM][0:NUM])
map(b[0:NUM][0:NUM]) map(c[0:NUM][0:NUM])
{
   #pragma omp parallel for collapse (2)
   for(i=0; i<msize; i++) {
      for(k=0; k<msize; k++) {
         #pragma omp simd
         for(j=0; j<msize; j++) {
            c[i][j] = c[i][j] + a[i][k] * b[k][j];
         }
      }
   }
}
```

Offloading – OMP Target Data



pragma OMP target data

```
#pragma omp target data map(to:a[0:NUM][0:NUM]) map(i , j ,k)
map(to:b[0:NUM][0:NUM]) map(tofrom:c[0:NUM][0:NUM])
{
   #pragma omp target
   {
      #pragma omp parallel for collapse (2) for(i=0; i<msize; i++) {
      for(k=0; k<msize; k++) {
         #pragma omp simd
         for(j=0; j<msize; j++) {
            c[i][j] = c[i][j] + a[i][k] * b[k][j];
         }
      }
   }
}
```

pragma OMP target update

- Update Data between host and device

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

- Clauses
```
device(scalar-integer-expression)
map(alloc | to | from | tofrom: list)
if(scalar-expr)
```

pragma OMP target update

```
#pragma omp target data map(to:a[0:NUM][0:NUM]) map(i , j ,k)
map(to:b[0:NUM][0:NUM]) map(to:c[0:NUM][0:NUM])
{
  #pragma omp target
  {
    #pragma omp parallel for collapse (2)
    for(i=0; i<msize; i++) {
      for(k=0; k<msize; k++) {
        #pragma omp simd
        for(j=0; j<msize; j++) {
          c[i][j] = c[i][j] + a[i][k] * b[k][j];
        }
      }
    }
  }
  #pragma omp target update from(c[0:NUM][0:NUM])
}
```

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Thread League

- **omp teams:** creates a league of thread teams
  - #pragma omp teams [clause [[,] clause] . . .]
    - num_teams(amount) : define the amount of thread teams
    - thread_limit(limit) : define the highest amount of threads that can be created in each team;
- **omp distribute:** distributes a loop over the teams in the league
  - #pragma omp distribute [clause [[,] clause] . . .]
    - dist_schedule (static[block size]):

Thread League

```
#pragma omp target teams num_teams (2) thread_limit (6)
{
   int i , N, teams , idteam , idthread ; int sum; N=20;
   #pragma omp distribute parallel for reduction (+:sum)
    for ( i =0; i<N; i ++) sum += i ;
}
```

Example1

```
#pragma omp target teams num_teams (3) thread_limit (3)
{
   int i , N, teams , idteam , idthread ; int sum; N=20;
   #pragma omp distribute parallel for reduction (+:sum)
    for ( i =0; i<N; i ++) sum += i ;
}
```

Example2

***Thread League*– Example 1**

Team 0: Thread 0, Thread 1, Thread 2, Thread 3, Thread 4, Thread 5

Team 1: Thread 0, Thread 1, Thread 2, Thread 3, Thread 4, Thread 5

0	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**	**13**	**14**	**15**	**16**	**17**

Logical Cores

***Thread League*– Example 2**

Team 0: Thread 0, Thread 1, Thread 2

Team 1: Thread 0, Thread 1, Thread 2

Team 2: Thread 0, Thread 1, Thread 2

0	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**	**13**	**14**	**15**	**16**	**17**

Logical Cores

Thread League – Example 1

```
#pragma omp target teams num_teams (2) thread_limit( 3 )
{
   int i, N, teams, idteam , idthread;
   int sum;
  N=20;

   #pragma omp distribute parallel for reduction (+: sum)
   for ( i =0; i <N; i ++) {
      sum += i ;
      idthread = omp_get_thread_num ();
      idteam = omp_get_team_num () ;
      teams = omp_get_num_teams () ;
      printf("i %d n %d idteam %d idthread %d teams %d \ n" , i ,N, idteam ,
idthread , teams ) ;
   }
}
```

Thread League – Example 2

```
#pragma omp target data device (0) map (i , j , k) map ( to : a[0:NUM]
[0:NUM] ) map ( to : b [ 0 :NUM] [ 0 :NUM] ) map ( tofrom : c [ 0 :NUM] [ 0
:NUM] )
{
   #pragma omp target teams distribute parallel for collapse (2) num_teams
(2) thread_limit (30)
   for ( i =0; i <NUM; i ++) {
      for ( k =0; k<NUM; k++) {
         #pragma omp simd
         for ( j =0; j <NUM; j ++) {
            c[i][j] = c[i][j] + a [i][k]  b[k][j] ;
         }
      }
   }
}
```

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N-Body

- An N-body simulation **[1]** aims at approximate the motion of particles that interact with each other according to some physical force;

- Used to study the movement of bodies such as satellites, planets, stars, galaxies, etc., which interact with each other according to the gravity force;

- Newton´s second law of motion can be used in in a N-body simulation to define bodies movement.

[1] AARSETH, S. J. Gravitational n-body simulations. [S.l.]: Cambridge University Press, 2003. Cambridge Books Online.

N-Body Algorithm

- Bodies struct:
  - 3 matrix represents velocity (x,y and z);
  - 3 matrix represents position (x,y and z);
  - 1 matrix represent mass;

- A loop calculate temporal steps:
  - In each temporal step new velocity and position are calculated to all bodies according to a function that implements Newton´s second law of motion;

N-Body – Parallel Version (host only)

```
function Newton(step)
{
   #pragma omp for
   for each body[x] {
      #pragma omp simd
      for each body[y]
         calc force exerted from body[y] to body[x];
      calc new velocity of body[x]
    }
    #pragma omp simd
    for each body[x]
       calc new position of body[x]
}

Main() {
   for each temporal step
      Newton(step)
}
```

N-Body – Parallel Version (Load Balancing)

- The temporal step loop remains sequential;
- The bodies are divided among host and devices to be executed using Newton;
- OpenMP Offload Pragmas are used to
  - Newton function offloading to devices;
  - Transfer data (bodies) between host and devices;

N-Body – Parallel Version (Load Balancing)

```
function Newton(step, begin_body, end_body, deviceId)
{
   #pragma omp target device (deviceId)  {
      #pragma omp for
      for each body[x] from subset(begin_body, end_body) {
         #pragma omp simd
         for each body[y] from subset(begin_body, end_body)
            calc force exerted from body[y] to body[x];
         calc new velocity of body[x]
      }
      #pragma omp simd
      for each body[x]
          calc new position of body[x]
   }
}
```

N-Body – Parallel Version (Load Balancing)

for each temporal step

Divide the amount of bodies among host and devices;

#pragma omp parallel

{

#pragma omp target data device (tid) to(bodies[begin_body: end_body])

{

Newton(step, begin_body, end_body, deviceId)

#pragma omp target update device (tid) (from:bodies)

#pragma omp barrier

#pragma omp target data device (tid) to(bodies[begin_body: end_body])

}

}