Advanced OpenMP Topics

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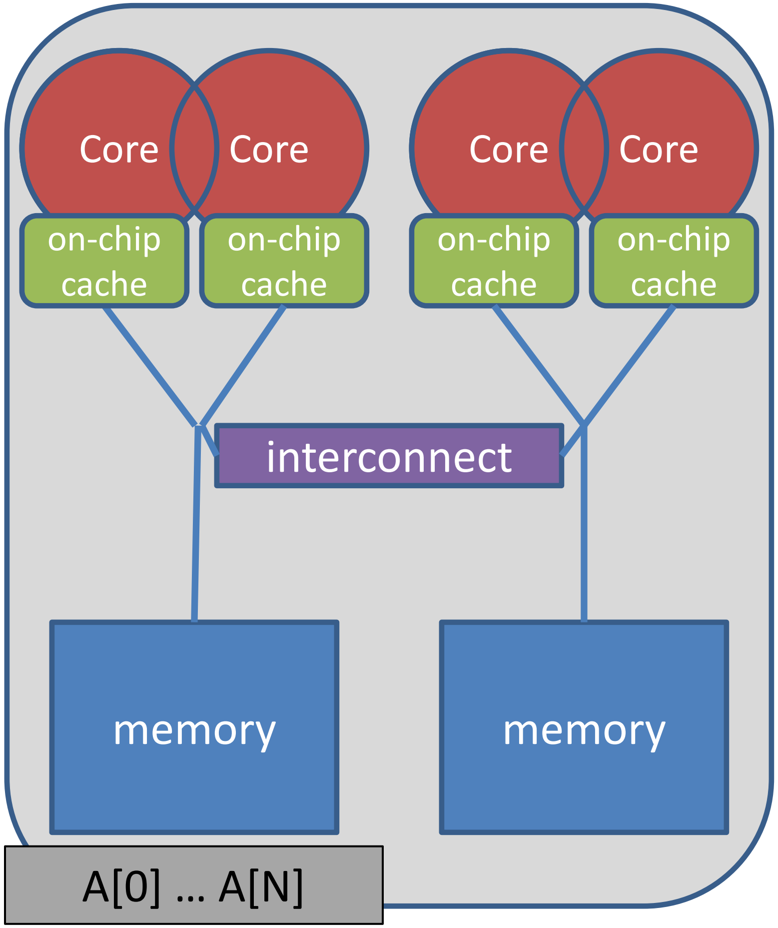
NUMA Architectures

How To Distribute The Data ?

```
double* A;
A = (double*)
     malloc(N * sizeof(double));


for (int i = 0; i < N; i++) {
   A[i] = 0.0;
}
```



About Data Distribution

- **Important aspect on cc-NUMA systems**
  - → If not optimal, longer memory access times and hotspots
- **OpenMP does not provide support for cc-NUMA**
- **Placement comes from the Operating System**
  - → This is therefore Operating System dependent

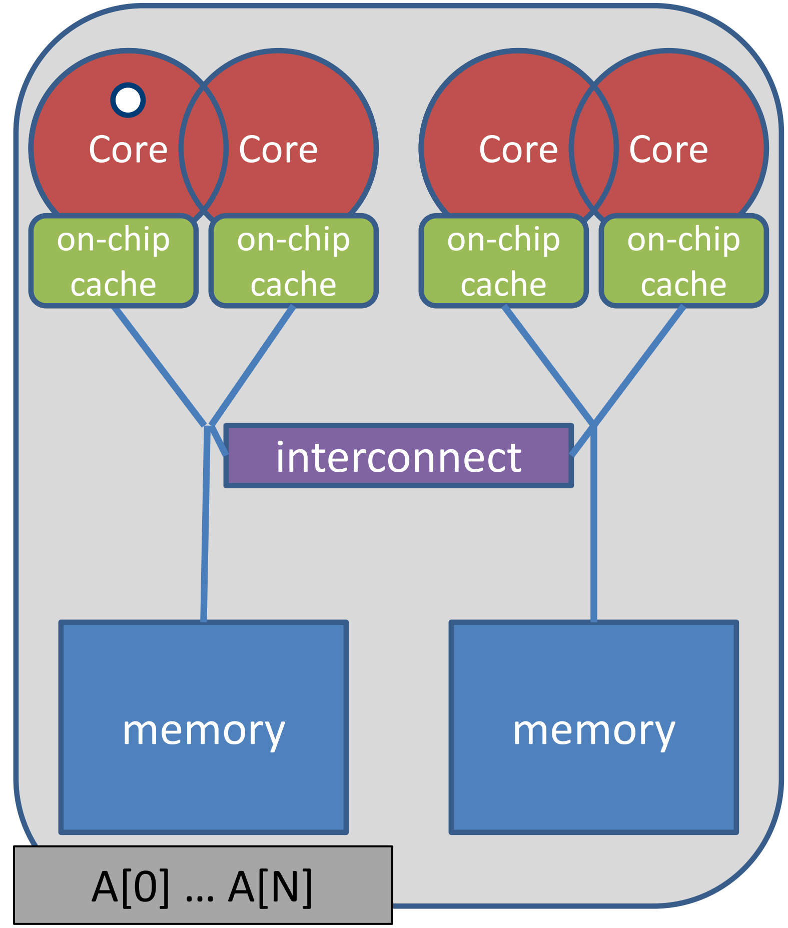
- **Windows, Linux and Solaris all use the “First Touch” placement policy by default**
  - → May be possible to override default (check the docs)

Non-Uniform Memory Arch.

- **Serial code: all array elements are allocated in the memory of the NUMA node containing the core executing this thread**

```
double* A;
A = (double*)
    malloc(N * sizeof(double));

for (int i = 0; i < N; i++) {
   A[i] = 0.0;
}
```



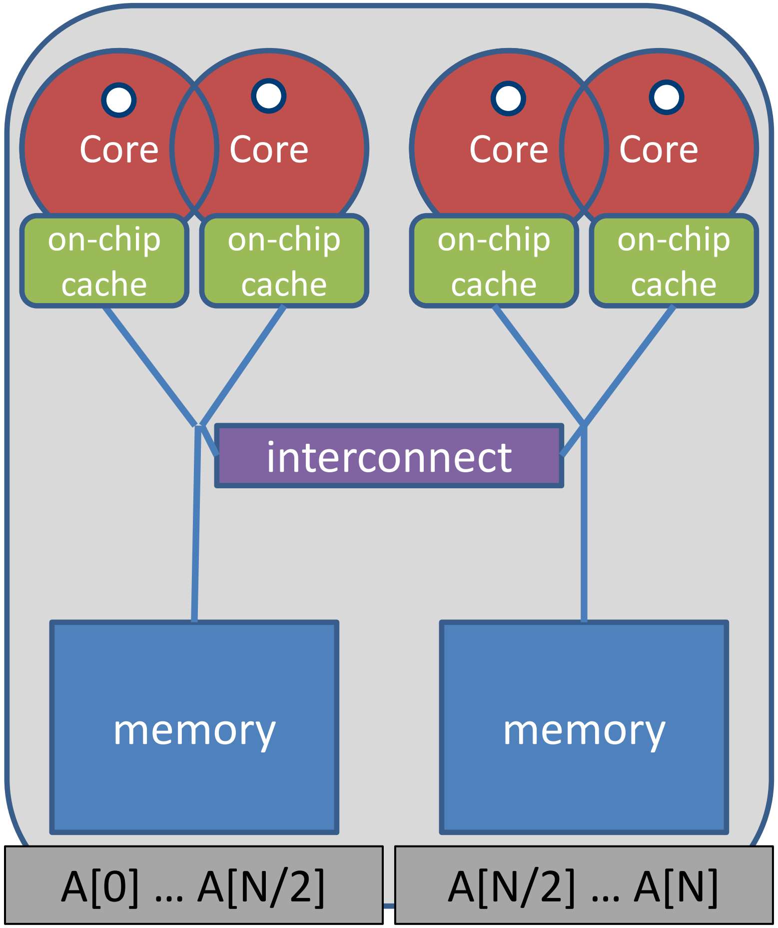
Non-Uniform Memory Arch.

- **First Touch w/ parallel code: all array elements are allocated in the memory of the NUMA node containing the core executing the thread initializing the respective partition**

```
double* A;
A = (double*)
    malloc(N * sizeof(double));

omp_set_num_threads(4);

#pragma omp parallel for
for (int i = 0; i < N; i++) {
   A[i] = 0.0;
}
```



Get Info on the System Topology

- **Before you design a strategy for thread binding, you should have a basic understanding of the system topology. Please use one of the following options on a target machine:**
  - → Intel MPI's `cpuinfo` tool
    - → `module switch openmpi intelmpi`
    - → `cpuinfo`
    - → Delivers information about the number of sockets (= packages) and the mapping of processor ids used by the operating system to cpu cores.
  - → hwlocs'tools
    - → `lstopo` (command line: `hwloc-ls`)
    - → Displays a graphical representation of the system topology, separated into NUMA nodes, along with the mapping of processor ids used by the operating system to cpu cores and additional info on caches.

Decide for Binding Strategy

- **Selecting the „right“ binding strategy depends not only on the topology, but also on the characteristics of your application.**
  - → Putting threads far apart, i.e. on different sockets
    - → May improve the aggregated memory bandwidth available to your application
    - → May improve the combined cache size available to your application
    - → May decrease performance of synchronization constructs
  - → Putting threads close together, i.e. on two adjacent cores which possibly shared some caches
    - → May improve performance of synchronization constructs
    - → May decrease the available memory bandwidth and cache size
- **If you are unsure, just try a few options and then select the best one.**

OpenMP 4.0: Places + Binding Policies (1/2)

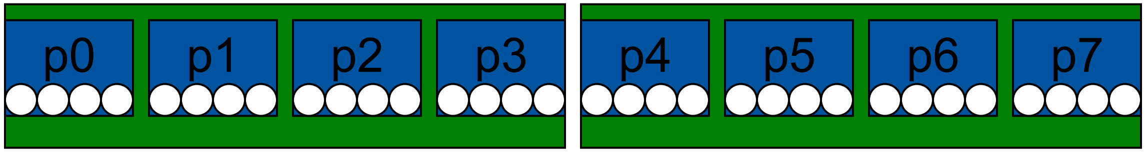
- **Define OpenMP Places**
  - → set of OpenMP threads running on one or more processors
  - → can be defined by the user, i.e. `OMP_PLACES=cores`

- **Define a set of OpenMP Thread Affinity Policies**
  - → SPREAD: spread OpenMP threads evenly among the places
  - → CLOSE: pack OpenMP threads near master thread
  - → MASTER: collocate OpenMP thread with master thread

- **Goals**
  - → user has a way to specify where to execute OpenMP threads for
  - → locality between OpenMP threads / less false sharing / memory bandwidth

Places

- **Assume the following machine:**



→ 2 sockets, 4 cores per socket, 4 hyper-threads per core

- **Abstract names for OMP_PLACES:**

→ threads: Each place corresponds to a single hardware thread on the target machine.

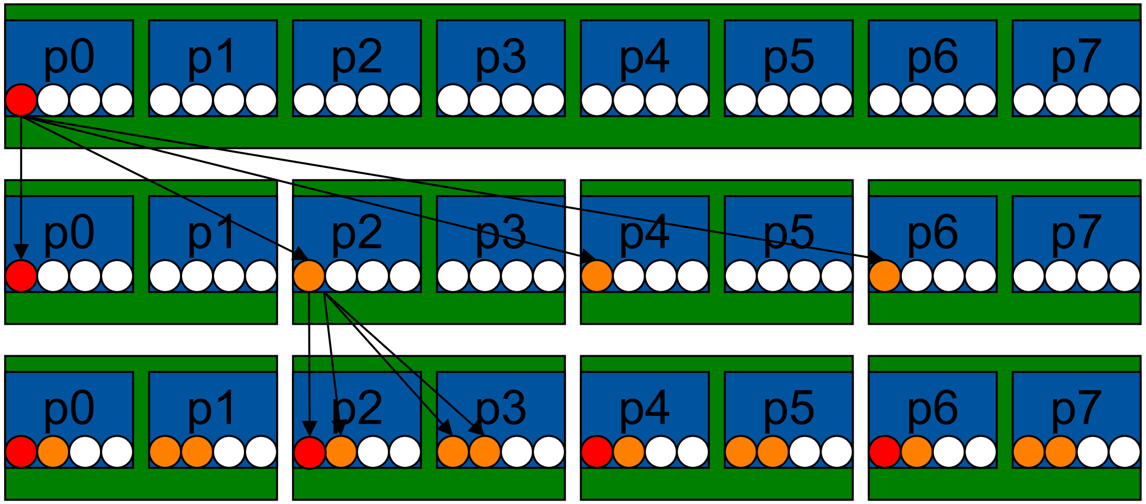
→ cores: Each place corresponds to a single core (having one or more hardware threads) on the target machine.

→ sockets: Each place corresponds to a single socket (consisting of one or more cores) on the target machine.

- **Example's Objective:**
  - → separate cores for outer loop and near cores for inner loop
- **Outer Parallel Region: proc_bind(spread), Inner: proc_bind(close)**
  - → spread creates partition, compact binds threads within respective partition

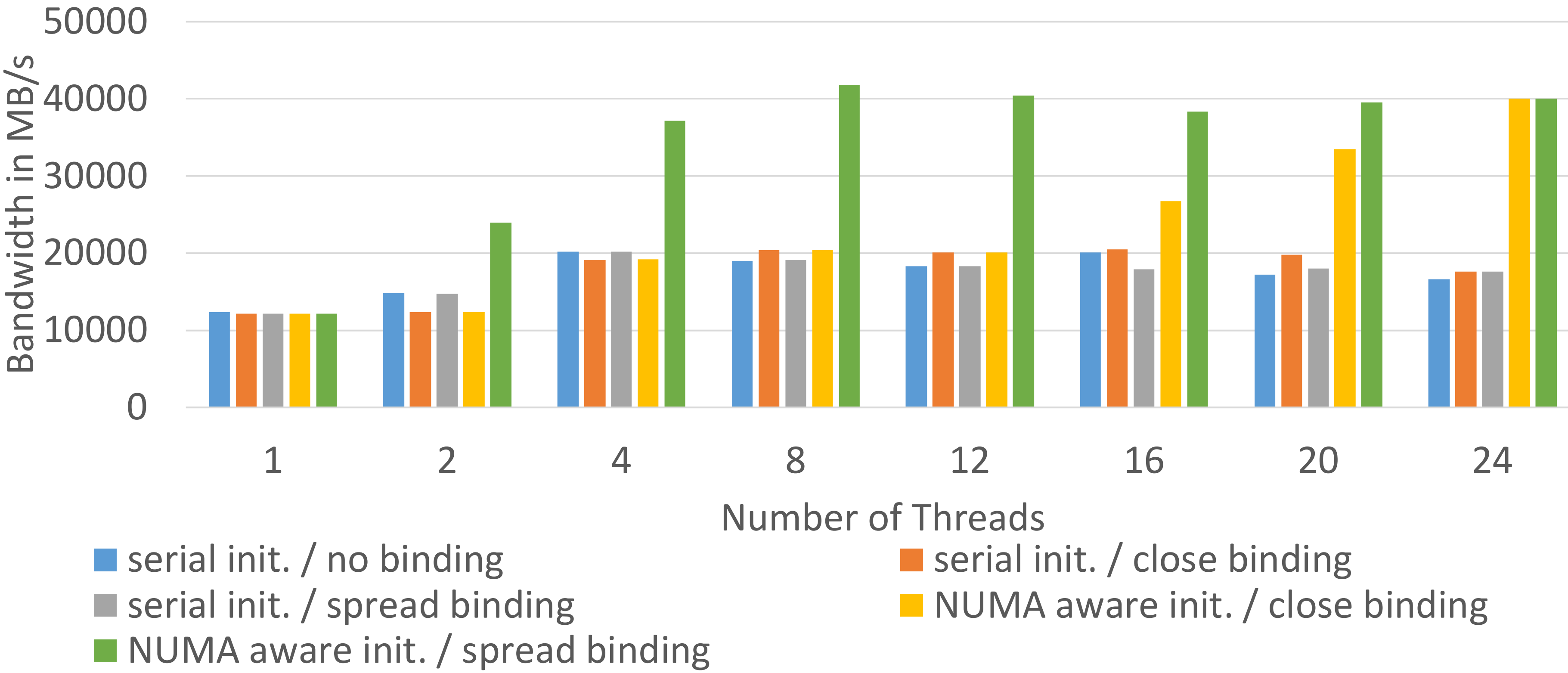
```
OMP_PLACES=(0,1,2,3), (4,5,6,7), ... = (0-3):8:4    = cores
#pragma omp parallel proc_bind(spread) num_threads(4)
#pragma omp parallel proc_bind(close) num_threads(4)
```

- **Example**
  - → initial
  - → spread 4
  - → close 4



Serial vs. Parallel Initialization

- **Performance of OpenMP-parallel STREAM vector assignment measured on 2-socket Intel® Xeon® X5675 („Westmere“) using Intel® Composer XE 2013 compiler with different thread binding options:**



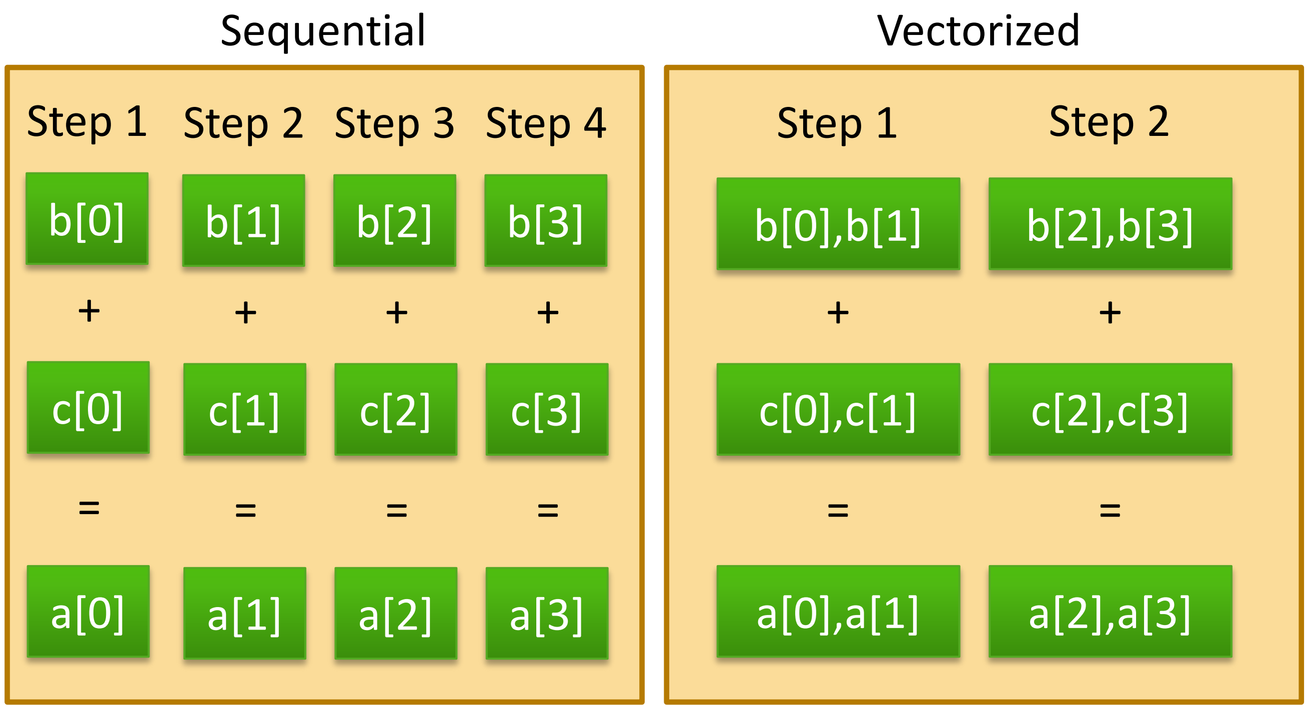
Vectorization (SIMD)

Vectorization

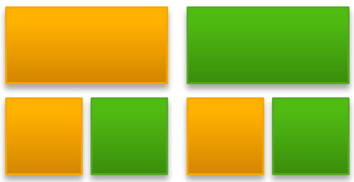
- **SIMD = S**ingle **I**nstruction **M**ultiple **D**ata
  - → Special hardware instructions to operate on multiple data points at once
  - → Instructions work on vector registers
  - → Vector length is hardware dependent

```
double a[4],b[4],c[4];
…

for(i=0 ; i < 4 ; i++)
{
        a[i]=b[i]+c[i];
}
```



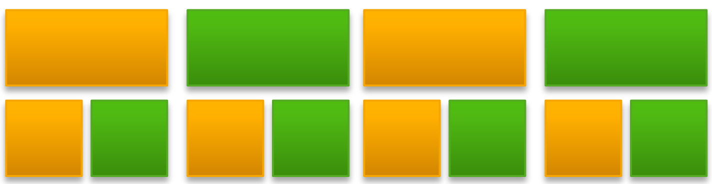
- **Vector lengths on Intel architectures**
  - → 128 bit: SSE = Streaming SIMD Extensions



2 x double

4 x float

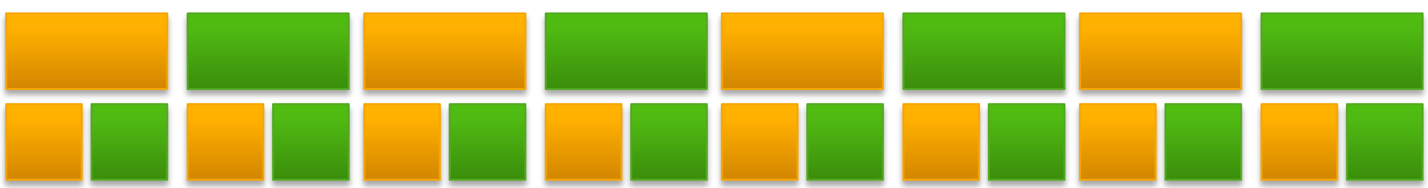
  - → 256 bit: AVX = Advanced Vector Extensions



4 x double

8 x float

  - → 512 bit: AVX-512

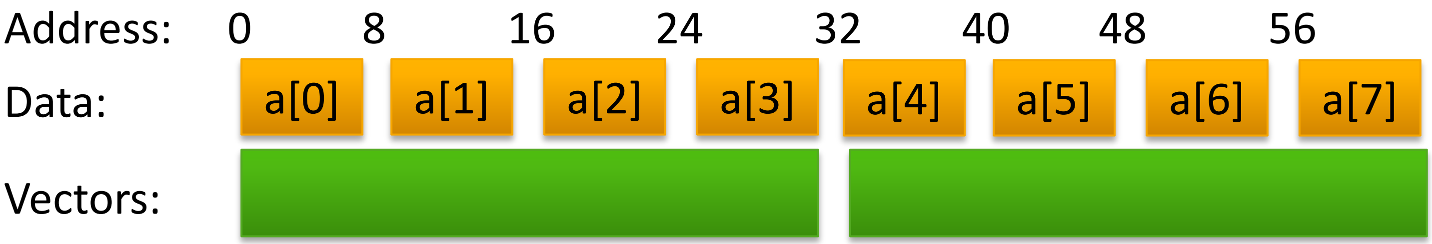


8 x double

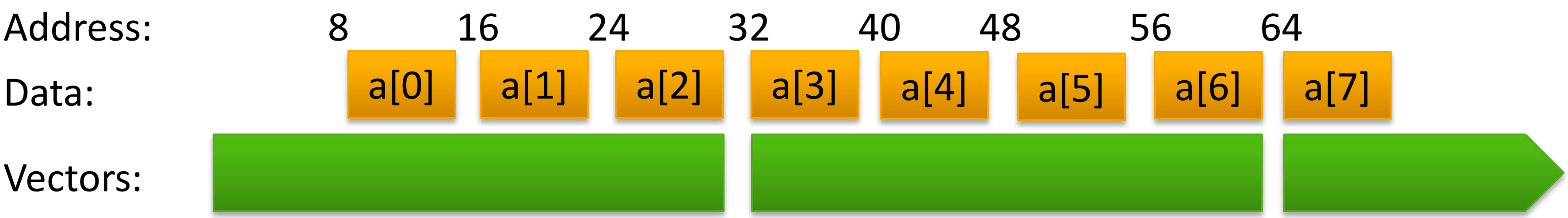
16 x float

- **Vectorization works best on aligned data structures.**

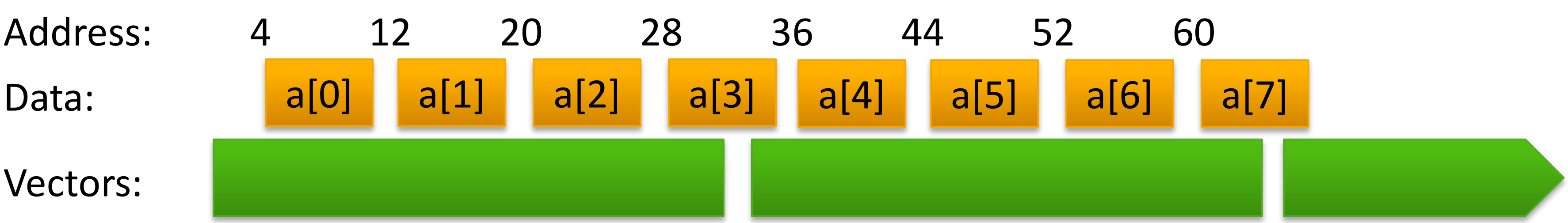
Good alignment



Bad alignment



Very bad alignment



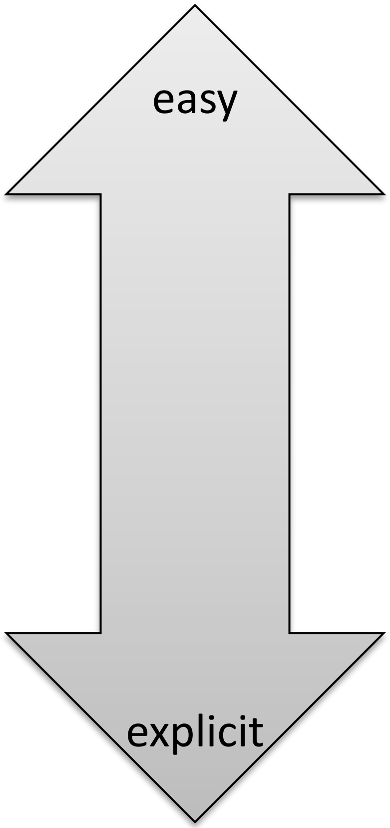
Ways to Vectorize

Compiler
auto-vectorization

Explicit Vector Programming
(e.g. with OpenMP)

Inline Assembly
(e.g.)

Assembler Code
(e.g. addps, mulpd, …)



The OpenMP SIMD constructs

The SIMD construct

- **The SIMD construct enables the execution of multiple iterations of the associated loops concurrently by means of SIMD instructions.**

```
C/C++:
#pragma omp simd [clause(s)]
  for-loops
```

```
Fortran:
!$omp simd [clause(s)]
  do-loops
[!$omp end simd]
```

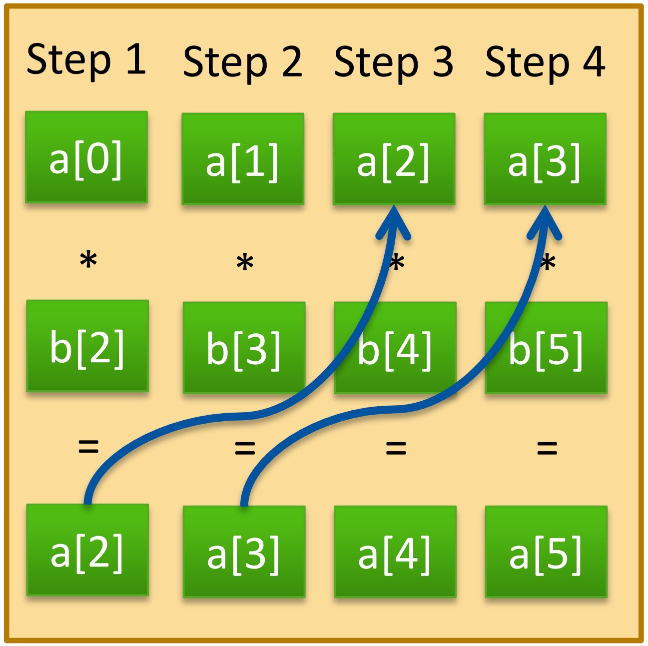
- **where clauses are:**
  - → linear(*list[:linear-step]*), a variable increases linearly in every loop iteration
  - → aligned(*list[:alignment]*), specifies that data is aligned
  - → private(*list*), as usual
  - → lastprivate(*list*) , as usual
  - → reduction(*reduction-identifier:list*) , as usual
  - → collapse(*n*), collapse loops first, and than apply SIMD instructions

- **The safelen clause allows to specify a distance of loop iterations where no dependencies occur.**

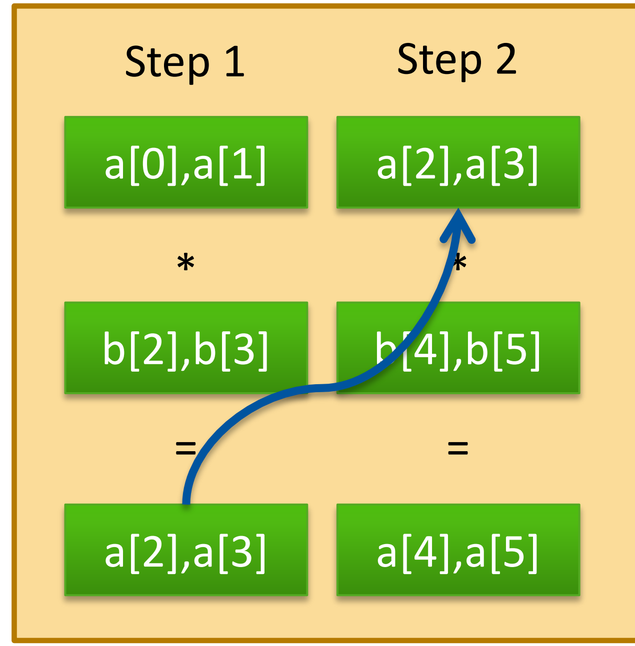
```
double a[6],b[6];
…

for(i=2 ; i < 6 ; i++)
{
      a[i]=a[i-2]*b[i];
}
```

Sequential



Vector length 128-bit

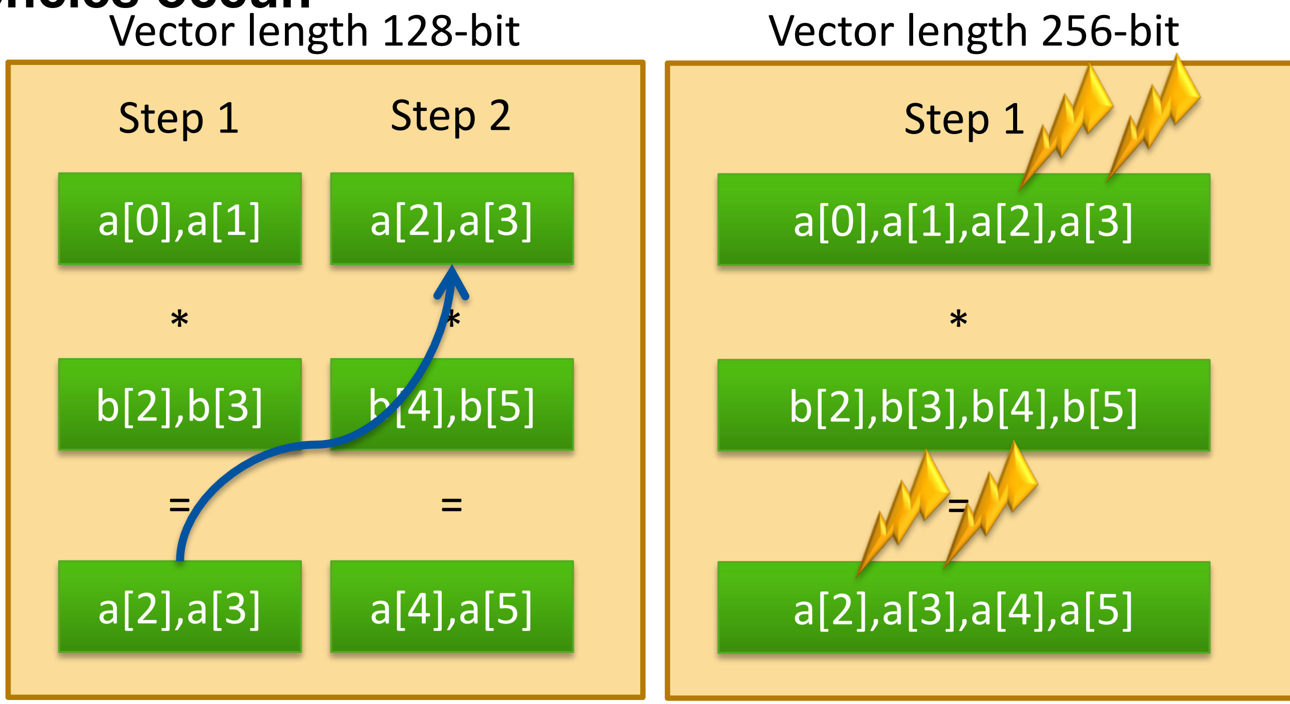


The SIMD construct

- **The safelen clause allows to specify a distance of loop iterations where no dependencies occur.**

```
double a[6],b[6];
…

for(i=2 ; i < 6 ; i++)
{
      a[i]=a[i-2]*b[i];
}
```



- **Any vector length smaller than or equal to the length specified by safelen can be chosen for vectorizaion.**
- **In contrast to parallel for/do loops the iterations are executed in a specified order.**

The loop SIMD construct

- **The loop SIMD construct specifies a loop that can be executed in parallel by all threads and in SIMD fashion on each thread.**

C/C++:
```
#pragma omp for simd [clause(s)]
  for-loops
```

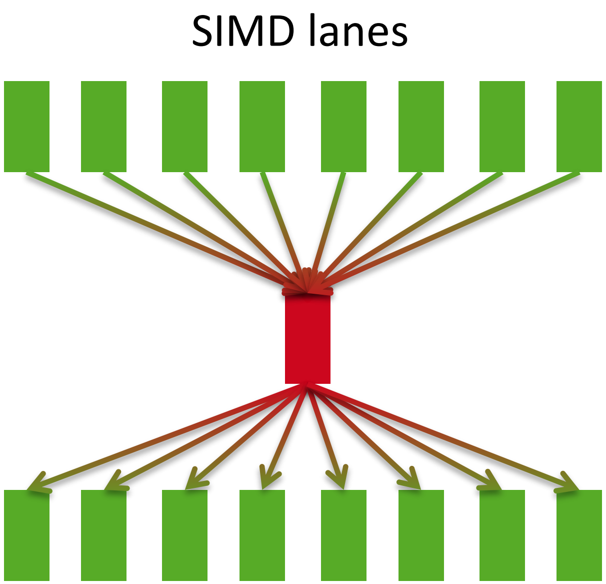
Fortran:
```
!$omp do simd [clause(s)]
  do-loops
[!$omp end do simd [nowait]]
```

- **Loop iterations are first distributed across threads, then each chunk is handled as a SIMD loop.**
- **Clauses:**
  - → All clauses from the *loop*- or SIMD-construct are allowed
  - → Clauses which are allowed for both constructs are applied twice, once for the threads and once for the SIMDization.

The declare SIMD construct

- **Function calls in SIMD-loops can lead to bottlenecks, because functions need to be executed serially.**

```
for(i=0 ; i < N ; i++)
{
      a[i]=b[i]+c[i];
      d[i]=sin(a[i]);
      e[i]=5*d[i];
}
```



Solutions:
- avoid or inline functions
- create functions which work on vectors instead of scalars

The declare SIMD construct

- **Enables the creation of multiple versions of a function or subroutine where one or more versions can process multiple arguments using SIMD instructions.**

C/C++:

```
#pragma omp declare simd [clause(s)]
[#pragma omp declare simd [clause(s)]]
  function definition / declaration
```

Fortran:

```
!$omp declare simd (proc_name)[clause(s)]
```

- **where clauses are:**
  - → simdlen(*length*), the number of arguments to process simultanously
  - → linear(*list[:linear-step]*), a variable increases linearly in every loop iteration
  - → aligned(*argument-list[:alignment]*), specifies that data is aligned
  - → uniform(*argument-list*), arguments have an invariant value
  - → inbranch / notinbranch, function is always/never called from within a conditional statement

File: f.c

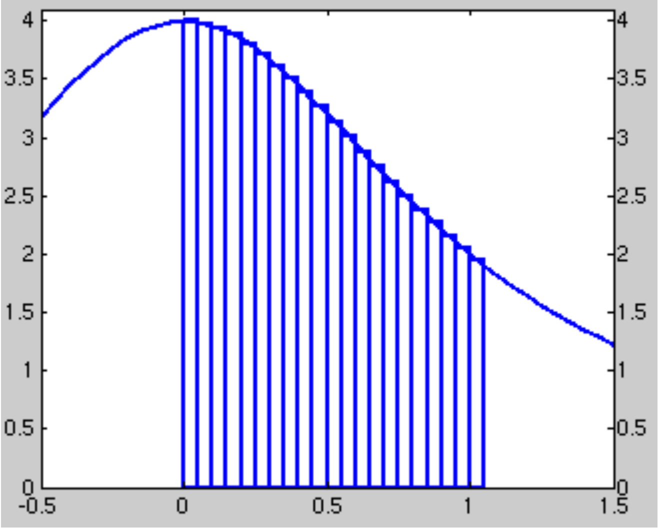
```
#pragma omp declare simd
double f(double x)
{
   return (4.0 / (1.0 + x*x));
}
```

File: pi.c

```
#pragma omp declare simd
double f(double x);
...
#pragma omp simd linear(i) private(fX) reduction(+:fSum)
for (i = 0; i < n; i++)
{
   fX = fH * ((double)i + 0.5);
   fSum += f(fX);
}
return fH * fSum;
```

Calculating Pi with numerical integration of:

$$\pi = \int_0^1 \frac{4}{1+x^2}$$



Example: Pi

- **Runtime of the benchmark on:**
  - → Westmere CPU with SSE (128-bit vectors)
  - → Intel Xeon Phi with AVX-512 (512-bit vectors)

	Runtime Westmere	Speedup Westmere	Runtime Xeon Phi	Speedup Xeon Phi
non vectorized	1.44 sec	1	16.25 sec	1
vectorized	0.72 sec	2	1.82 sec	8.9

Note: Speedup for memory bound applications might be lower on both systems.

Questions?