



# Introduction to OpenMP

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## How to build faster computers – a survey



## 1. Increase performance / throughput of CPU core

- a) Reduce cycle time, i.e. increase clock speed (Moore)
- b) Increase throughput, i.e. superscalar + SIMD

## 2. Improve data access time

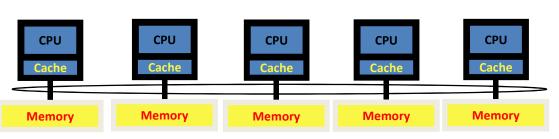
- a) Increase cache size
- b) Improve main memory access (bandwidth & latency)

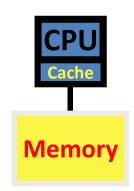
## 3. Use parallel computing (shared memory)

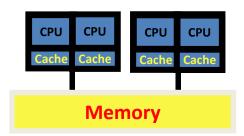
- a) Requires shared-memory parallel programming
- b) Shared/separate caches
- c) Possible memory access bottlenecks

# 4. Use parallel computing (distributed memory) "Cluster" of computers tightly connected

- a) Almost unlimited scaling of memory and performance
- b) Distributed-memory parallel programming







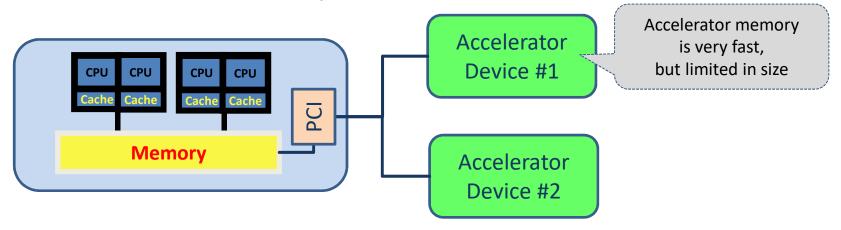


## How to build faster computers (cont'd)



## 5. Use an accelerator with your compute node

- Requires offload of program regions as well as data (semantics may be limited)
- b) Host and accelerator memory are connected, but separate



(Improvements are under way)

 Programming complexity is higher than for shared memory systems ("heterogeneous parallel computing")



## **Multi-core processor**

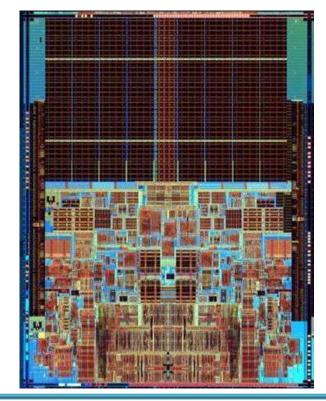


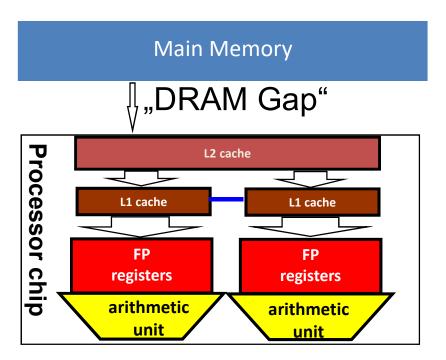
It is not a faster CPU – it is a parallel computer on a chip.

Put multiple processors ("cores") on a chip which share resources (example shows a dual core that shares L2 cache and memory bandwidth)

Efficient use of all cores for a single application → programmer

Intel Xeon (Woodcrest)



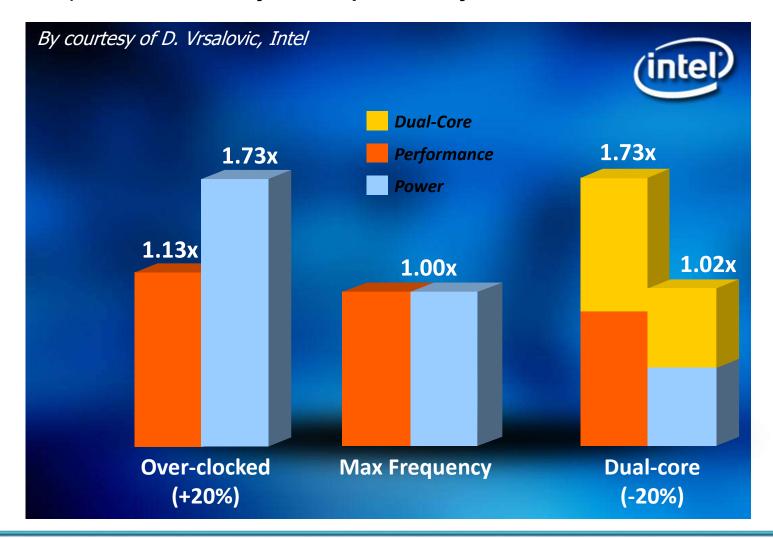




# ... the party is over!



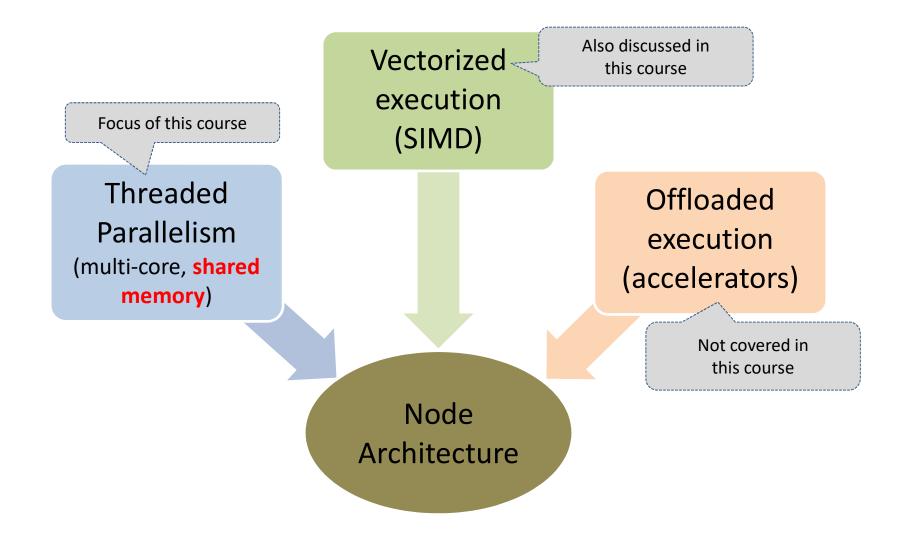
Option 1 a) is not feasible any more, option 2 only in small increments





# Paradigms supported by OpenMP – three faces of parallelism







## **OpenMP** and portability



### Syntactic portability

- Directives / pragmas
- Conditional compilation permits to mask API calls

## Semantic portability

- Standardized across platforms
   → safe-to-use interface
- Unsupported/unavailable hardware features → irrelevant directives will be ignored (you might need a special compiler for your devices ...)

### Performance portability

- Unfortunately, performance is not necessarily portable
- Has traditionally been a problem (partly due to differences in hardware/architectural properties)
- Becoming worse with recent hardware generations



## **Compatibility with Sequential Execution**



#### **Are semantics for sequential execution retained?**

- yes, due to directive concept
- programmer may choose not to

#### Do memory accesses occur in the same order?

 no, due to relaxed memory consistency (performance feature!)

#### Are the same numeric results obtained for parallel execution?

- no associativity for model number operations
- parallel execution might reorder operations (programmer may need to enforce ordering for reproducibility and/or numeric stability)



## **OpenMP Standard**



- Responsible body: OpenMP Architecture Review Board
  - Published OpenMP 5.0 in November 2018

Base languages

- Fortran (up to 2008)
- C, C++
- (Java is not a base language)

starts in 1997

History of OpenMP

Fortran and C examples will be displayed

#### Resources:

- <a href="http://www.openmp.org">http://www.openmp.org</a> (including standard documents)
- http://www.compunity.org

#### Note:

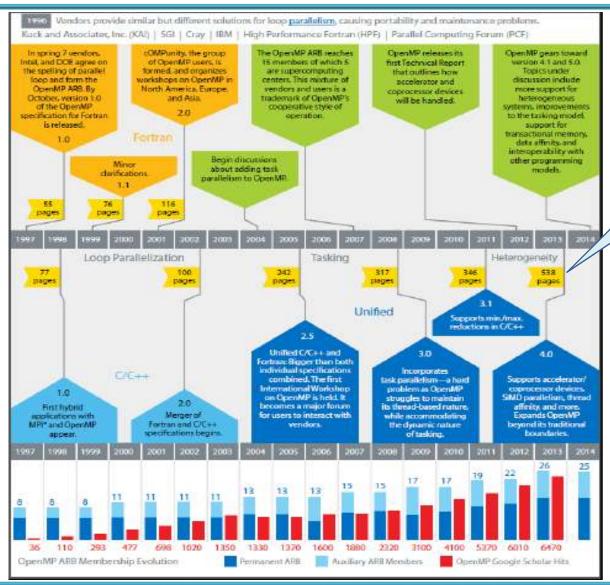
LRZ has become a member of the OpenMP ARB in March, 2019



## **OpenMP** history



(courtesy Intel "The Parallel Universe", issue 18)



Note the increase in the standard's size (OpenMP 5.0 has 666 pages)

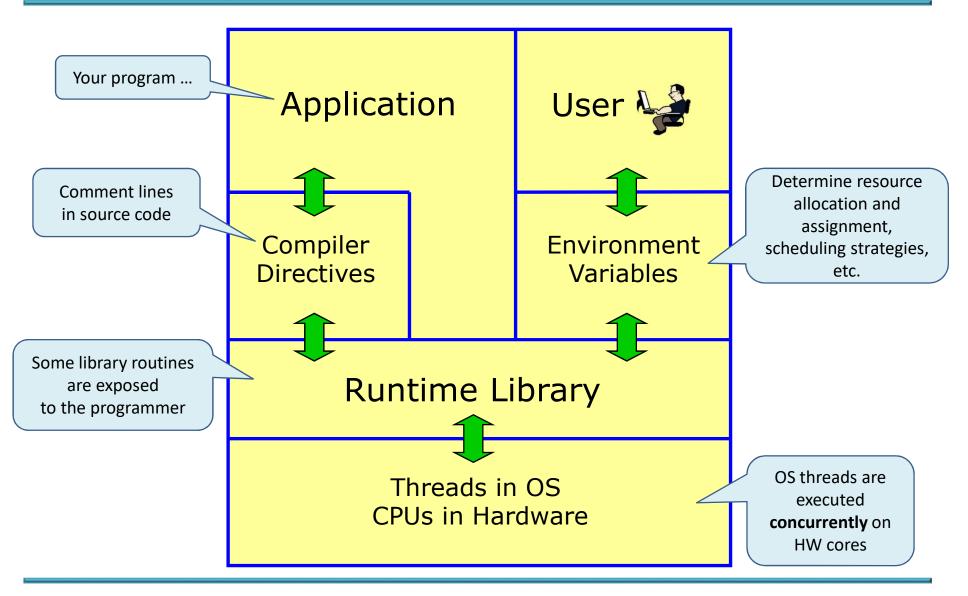
#### **Course Target:**

Learn the most useful and therefore most commonly used features of OpenMP



## **OpenMP Architecture**







## A simple application

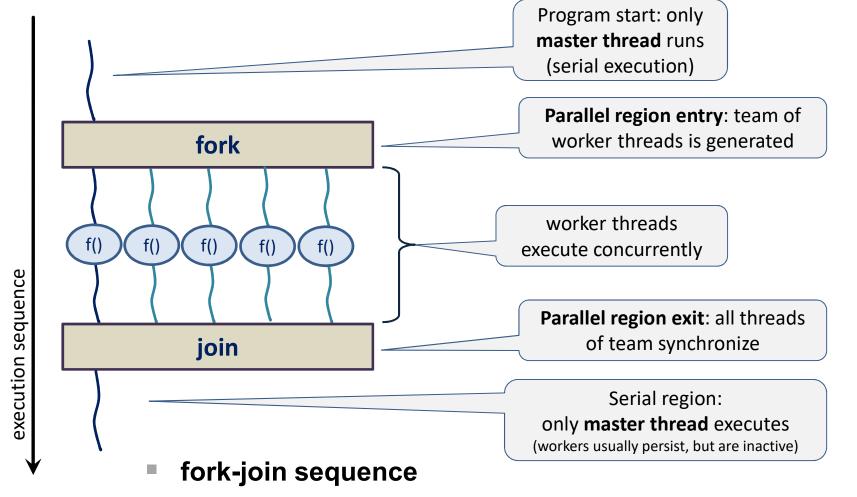


```
Fortran
                                  #include <stdio.h>
program
                                  int main() {
  use m
  implicit none
                    Aim is to execute
                   multiple instances of
                                    f();
  call f()
                     f() concurrently
                                     return 0;
end program
module m
  implicit none
contains
                                  void f() {
  subroutine f()
    print *, 'Hello'
                                     printf("Hello\n");
  end subroutine
end module
```



### Parallel execution model



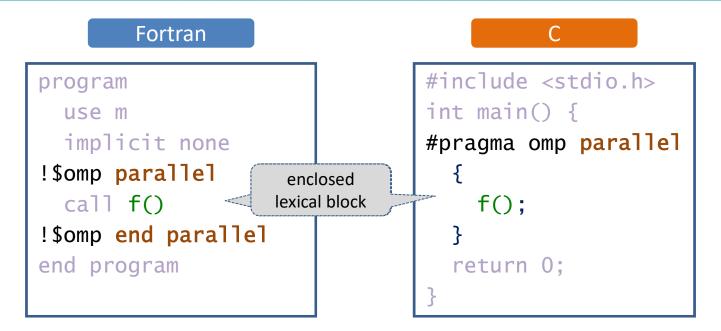


can repeat, with differing thread counts

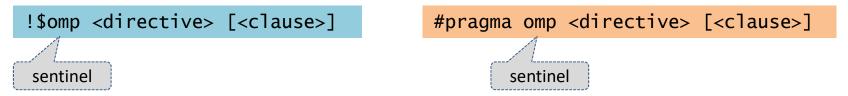


## Adding a parallel region

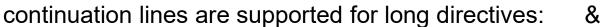




#### General form of directives:



- clauses, if present, modify a directive's semantics
- multiple clauses per directive are possible



Fortran



## **OpenMP structured block rules**



#### Fortran

 statements between a beginning and ending directive pair



 delineated by braces following a directive

#### single point of entry

GOTO into block is prohibited

setjmp() into block is prohibited

## single point of exit

 GOTO, RETURN, EXIT outside block are prohibited  longjmp() and throw() outside block are prohibited

#### permitted: program termination

STOP, ERROR STOP

exit()

# **Using library calls**



Fortran



## **Independent execution contexts**



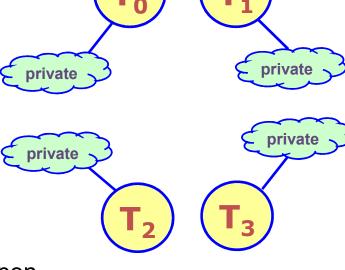
- As many independent function calls as there are threads
- Thread-individual memory management within function call
  - local variables (e.g., "me") are created in the thread-specific stack
  - malloc() or ALLOCATE create memory in the heap separately for each thread

#### Private variables

- associated with a particular thread are inaccessible by any other thread
- pro: safe to use
- con: communication is not possible
   (it is needed by many parallel algorithms),
   unnecessary replication of objects may happen.

#### Thread-individual stack limit

 control via environment variable (example: 100 MByte)



export OMP\_STACKSIZE=100M



subset

most commonly used

# **OpenMP API**



#### Classes of routines:

• Execution environment (36), Locking (12), Timing (2), Device Memory (7)

	Name	Result type	Purpose
	omp_set_num_threads (int num_threads)	none	number of threads to be created for subsequent parallel region
	<pre>omp_get_num_threads()</pre>	int	number of threads in currently executing region
	<pre>omp_get_max_threads()</pre>	int	maximum number of threads that can be created for a subsequent parallel region
	<pre>omp_get_thread_num()</pre>	int	thread number of calling thread (zero based) in currently executing region
l	<pre>omp_get_num_procs()</pre>	int	number of processors available
	<pre>omp_get_wtime()</pre>	double	return wall clock time in seconds since some (fixed) time in the past
	<pre>omp_get_wtick()</pre>	double	resolution of timer in seconds



# **Compiling and Running**



Compilation:

Fortran

f90 -fopenmp -o hello.exe hello.f90

generic instructions ...

С

cc -fopenmp -o hello.exe hello.c

- Switch for OpenMP
  - specific spelling is compiler-dependent
  - toggles both directives and conditional compilation
  - generates threaded code and links against OpenMP run time
- Execution:

```
export OMP_NUM_THREADS=4
./hello.exe
```

by default, parallel regions generate a team with 4 threads

serial compilation may

require stub library

Output for example program:

```
Hello from 1
Hello from 0
Hello from 2
```

ordering will vary between runs (asynchronous execution)

Now: First exercise session





# Simple work sharing, Scoping of Data, and Synchronization



## Questions that now arise ...



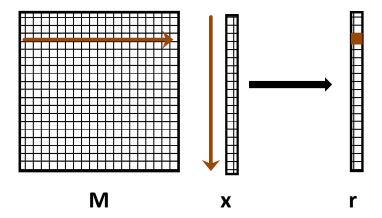
## We know how to set up threading, but

- how can a large work item be divided up among threads? (using the API for this works in principle, but is tedious)
- what happens with objects that already exist before the parallel region starts?

## **Example:**

$$r = M \cdot x$$
 i.e.

matrix-vector multiplication 
$$r = M \cdot x$$
 i.e.  $r_i = \sum_{j=1}^{n} M_{ij} x_j$ 



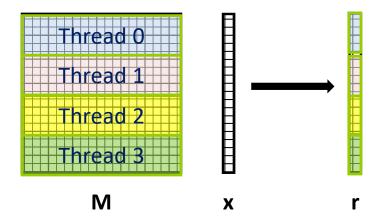
A bunch of scalar products



## **Concept of work sharing**



#### The idea is to split the work among threads



#### Note that

- all elements of x must be available to all threads
- Matrix-Vector is often deployed iteratively → r becomes x in the next iteration
   → copying of data must be possible

## Consequence:

- need for variables that are accessible to all threads
  - → "data sharing" is often a prerequisite for "work sharing"
  - → a natural concept for a shared memory programming model

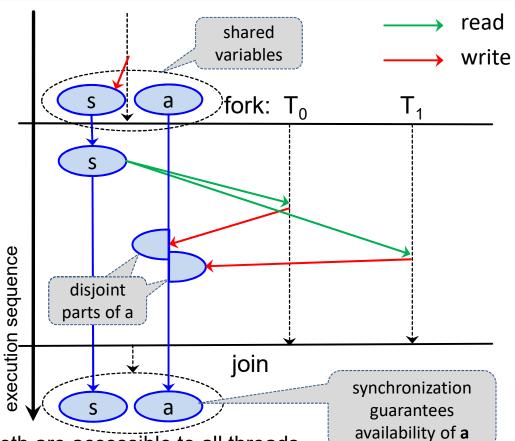


## **Sharing variables across threads**



```
real :: s, a(200) Fortran

s = ...
!$omp parallel shared(s,a)
select case (me) thread ID
case (0)
a(1:100) = ... * s
case (1)
a(101:200) = ... * (-s)
end select
!$omp end parallel
```



- The "shared" clause
  - implies that scalar **s** and array **a** both are accessible to all threads
- Rules for concurrent accesses to a single object
  - reads/writes or writes/writes by different threads are not permitted ("data races")

Note: updates to array a are OK because disjoint parts of object are updated



## Data dependencies that prevent parallelization



Flow dependency ("read after write", RAW):

Anti-dependency ("write after read", WAR):



resolvable at cost of introducing a new variable ("name dependency")

Output dependency ("write after write", WAW):

after name dependency resolution, statements 1 and 3 can execute concurrently.

Flow dependency remains.



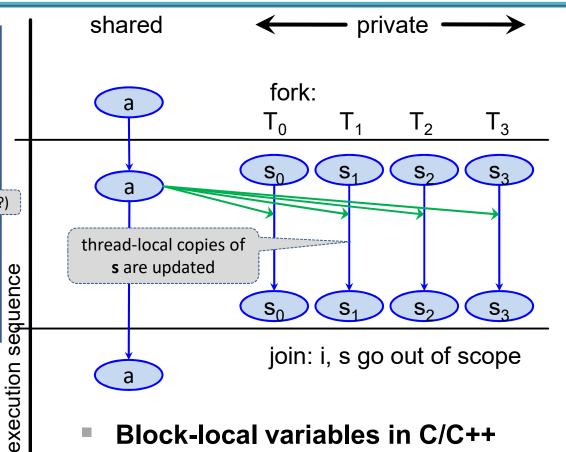
## **Privatization**



```
a[k] = ...;
#pragma omp parallel \
          shared(a)
  { int i; float s;
    s = 0.0; split iteration space (?)
     for (i=...;i<...;i++) {
       s += a[i];
                                sedneuce
```

example calculates thread-individual sums

useless, from a practical point of view. But bear with me we'll fix this, eventually



- **Block-local variables in C/C++** 
  - are automatically private

Note: One can expect the same behaviour for the Fortran 2008 BLOCK construct, but this is currently not specified in the OpenMP standard



## **Privatization with masking**

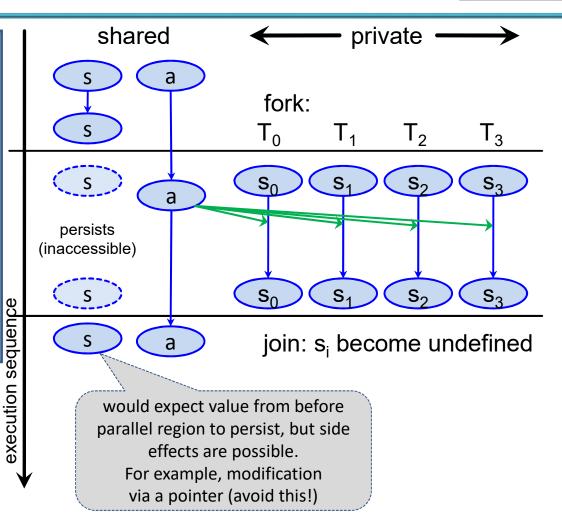


#### Masking occurs

 for privatized variables declared outside the parallel region

### Loop variables

are always private



• If **s** were shared, the program would have a race condition.



# Code for work-shared Matrix-Vector multiplication: The DO / FOR directive



#### Serial

#### Fortran

```
DO k = 1, n

DO j = 1, n

r(j) = r(j) + a(j, k) * x(k)

END DO

END DO
```

#### C

```
for (k=0; k<n; k++) {
   for (j=0; j<n; j++) {
     r[j] = r[j] + a[k*n+j] * x[k];
   }
}</pre>
```

## OpenMP parallel



## Further rules for work shared loops



### Slicing of iteration space

- "loop scheduling"
- default behaviour is implementation dependent
- usually as equal as possible chunks of largest possible size, one chunk per thread

## In the example,

- slicing is done as shown some slides earlier
- loop order was switched to avoid having many synchronizations

#### Additional clauses

 on OMP DO / omp for will be discussed later

#### Restrictions on loop structure

Trip count must be computable at entry to loop

#### • Disallowed:

C style loops modifying the loop variable in the loop body, or using a non-evaluable exit condition, or Fortran DO WHILE loop;

 loop body must be a well-formed structured block with single entry and single exit point

#### Note:

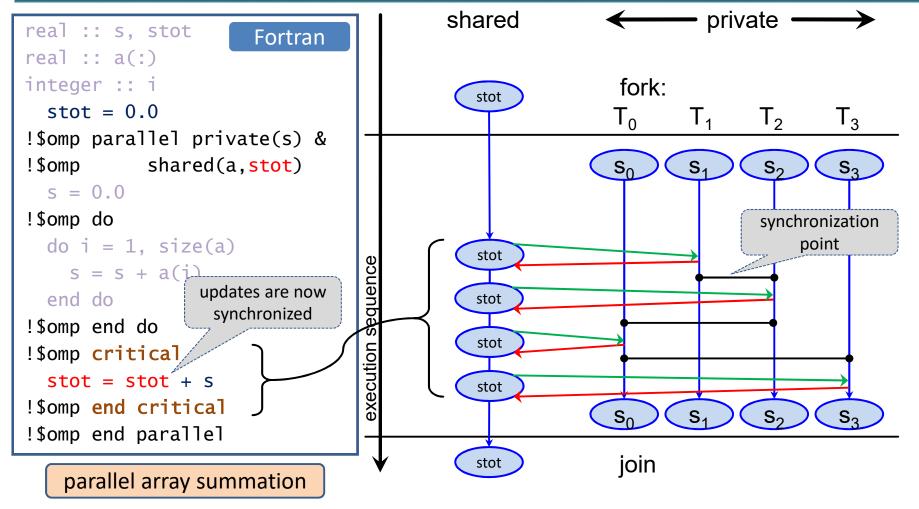
 directive (by default) acts only on outermost enclosed loop

actually, we're caught between a rock and a hard place here ...



# Avoiding race conditions (1): mutual exclusion via the critical directive





- Only one thread at a time can execute a critical region
  - others must wait → code in region is effectively serialized



# Dealing with race conditions through atomic updates



parallel array summation

## Properties of atomic operations

- the atomic directive applies only for a single update to a scalar shared variable of intrinsic type
- this way of updating can be done safely when executed concurrently (exception to the rules on race conditions!)
- otherwise, no synchronising effect imposed by semantics
- hardware atomic instructions available → likely more efficient than critical region

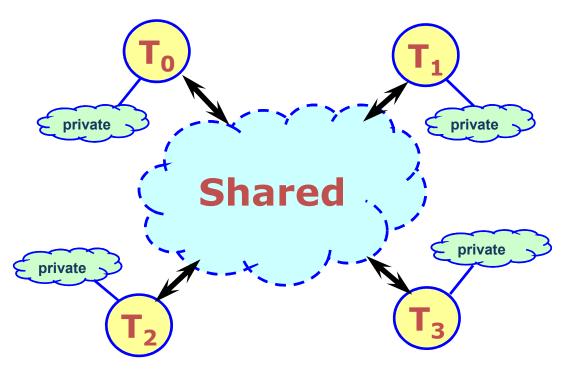
legacy notation omp atomic is also permitted

- C can use #pragma omp critical
- Fortran can use !\$omp atomic ...



## The two kinds of memory in OpenMP





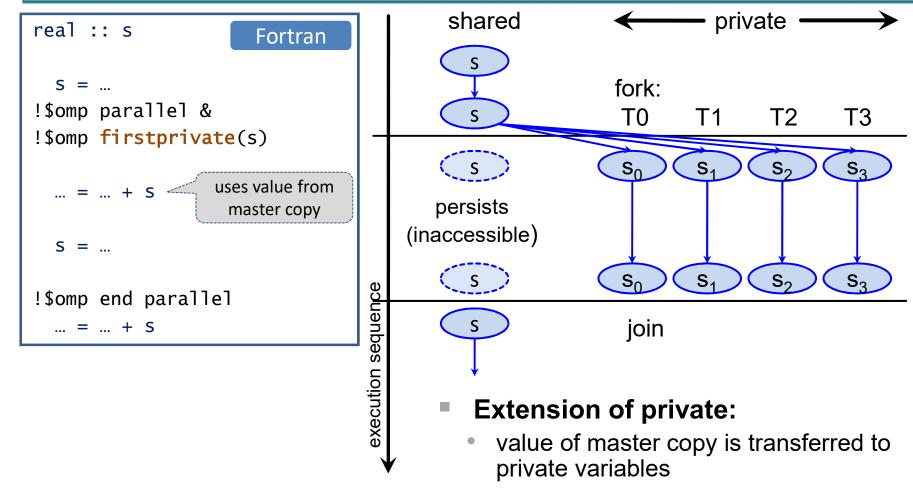
## Data accessed by can be shared or private

- shared data one instance of an entity available to all threads (in principle)
- private data each perthread copy only available to thread that owns it
- Data transfer transparent to programmer
- Synchronization necessary for accessing shared data from different threads to avoid race conditions
  - implicit barrier
  - explicit directive



## The firstprivate clause





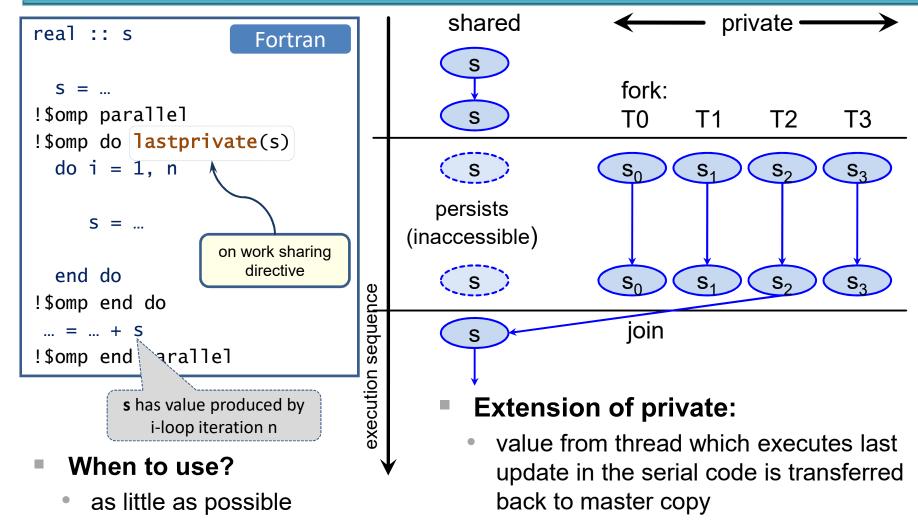
restrictions: not a pointer, not assumed shape, not a subobject, master

copy not itself private etc.



## The lastprivate clause





legacy code

restrictions similar to firstprivate



## **Data scoping defaults**



# Scoping clauses can be specified for

- parallel regions
- loop work sharing constructs

#### Defaults

- apply if no clause is specified
- may vary by construct, but for the above the following apply:

pre-existing objects are by default **shared**, except for loop variables, which are **private**.

objects declared inside the lexical or dynamic scope of the construct are **private**.

this cannot be changed, of course

#### Recommendation:

 specify a default(none) clause on each directive that permits scoping:

**Fortran** 

other values are possible

```
!$omp parallel default(none) &
!$omp shared(...) private(...) ...
...
```

С

```
#pragma omp parallel default(none) \
    shared(...) private(...) ...
```

this **forces** you to explicitly consider and specify scoping for all pre-existing objects

Now: Second exercise session



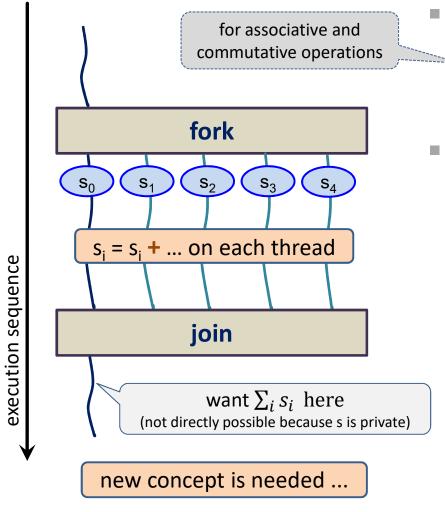


# Reductions



## **Concept of Reduction**



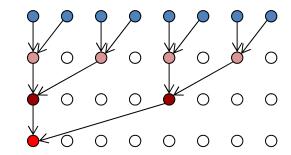


## Seen in previous exercise:

- need for assembling partial results across threads
- up to now: with critical region

## OpenMP reductions:

- sometimes more efficient at scale
- implementation tunings like



reduce complexity from  $O(n_{threads})$  to  $O(log_2(n_{threads}))$ 

always easier to understand and maintain



#### Reduction clause



#### Example 1: Sum reduction in a parallel region

```
real :: s

Fortran

s = 2.2 incoming value

!$omp parallel reduction(+:s)

s = s + ...

private copy of s
(initial value 0.0)

!$omp end parallel

s can be safely consumed due to previous implicit barrier
```

- value of s after end of parallel region:  $s_{incoming} + \sum_{i} s_{i}$
- Note: multiple reductions are permitted

```
!$omp parallel reduction(+:x,y,z)
!$omp parallel reduction(+:x,y) &
!$omp reduction(*,z)
```



#### Reduction clause cont'd



Example 2: Sum reduction in a work shared region

```
real :: s
                                         float s:
                       Fortran
                                         s = 2.2;
  s = 2.2 incoming value
                                       #pragma omp parallel shared(s)
!$omp parallel shared(s)
!$omp do reduction(+:s)
                                       #pragma omp for reduction(+:s)
                                           for (i=0, i<n, i++) {
  do i = 1, n
                        private copy of s
                                                        operation consistent
                        (initial value 0.0)
  end do
!$omp end do
  ... = ... * S
!$omp end parallel
                        s can be safely consumed due to
                           previous implicit barrier
```

• value of s after end of worksharing region:  $s_{incoming} + \sum_{i} s_{i}$ 



## Initial value of private reduction variables



- Depends on operation
- Supported intrinsic operations:

Fortran

Operation	Initial value		
+	0		
-	0		
*	1		
.and.	.true.		
.or.	.false.		
.eqv.	.true.		
.neqv.	.false.		
MAX	-HUGE(X)		
MIN	HUGE(X)		
IAND	all bits set		
IEOR	all bits 0		
IOR	all bits 0		

C / C++

Operation	Initial value
+	0
-	0
*	1
&	0
1	0
٨	0
&&	1
	0
MAX	smallest representable value
MIN	largest representable value



## **Array reductions**

now also supported in C/C++!



```
real :: a(*)
real :: b(n)

!$omp parallel reduction(+:b) &
!$omp reduction(*:a(1:m))
...

must specify
upper bound
(assumed size)
```

```
float *a;
float b[N];
pointee created
e.g. via malloc()

#pragma omp parallel \
reduction(+:b[:]) \
reduction(*:a[0:m])
...
```

- reduces complete array b and m elements of array a, elementwise
- uses regular Fortran array section notation

[lower bound : upper bound]

- C example does the same as the Fortran example
- OpenMP-defined sectioning syntax (differs from Fortran):

[lower bound : length]

#### General rules:

- array section must be a contiguous object (→ no strides permitted)
- dynamic objects must be associated / allocated, and the status must not be modified for the private copies



#### **User-defined reductions**



#### Using derived types

```
type :: fraction
integer :: numerator, denominator
end type

add overloaded operators +, -, * etc.
or even user-defined operators
```

#### And now we want to write

```
type(fraction) :: af
af = ...
!$omp parallel reduction(+:af)
...
af = af + ...
!$omp end parallel
```

```
typedef struct {
  int numerator, denominator;
} Fraction;

provide functions to add, etc.
```

 but the compiler will refuse to build it ("+" not known to OpenMP) unless further measures are taken ...



## Declaring a user-defined reduction



```
!$omp declare reduction(+:fraction:omp_out=omp_out+omp_in) &
!$omp
initializer(omp_priv=fraction(0,1))
```

Fortran

Combiner

declare reduction(<op>:<type>:<combiner>)

- connects to operator implementation
   Fortran: example defers to overloaded "+", C: references "Fraction\_add" special OpenMP parameters omp\_in, omp\_out formally describe the two operands for each operation needed
- Initializer

initializer(omp\_priv=...) or initializer(function(...))

implements initial value setting for private copies
 Fortran: uses (overloaded) structure constructor, C similar special OpenMP parameter omp\_priv formally describes private copy





## **More on Work Sharing**

Loops and loop scheduling
Collapsing loop nests
Parallel sections



#### The schedule clause



#### Default scheduling:

- implementation dependent
- **typical:** largest possible chunks of asequal-as-possible size ("static scheduling")

iteration space (threads color coded)

#### User-defined scheduling:

Fortran static
!\$OMP do schedule( dynamic [,chunk] )
guided

**chunk:** always a non-negative integer. If omitted, has a schedule dependent default value

#### 1. Static scheduling

schedule(static,10)



- minimal overhead (precalculate work assignment)
- default chunk value: see left

#### 2. Dynamic scheduling

 after a thread has completed a chunk, it is assigned a new one, until no chunks are left

schedule(dynamic, 10)



both threads take long to complete their chunk (workload imbalance)

- synchronization overhead
- default chunk value is 1



## 3. Guided scheduling



#### Size of chunks in dynamic schedule

- too small → large overhead
- too large → load imbalance
- Guided scheduling: dynamically vary chunk size.
  - Size of each chunk is proportional to the number of unassigned iterations divided by the number of threads in the team, decreasing to chunk-size. (default: → 1)

#### Chunk size:

- means minimum chunk size (except perhaps final chunk)
- default value is 1

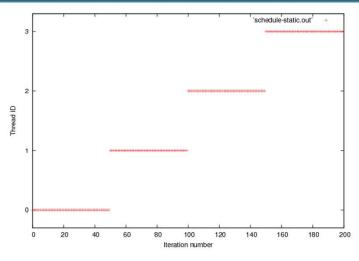


 both dynamic and guided scheduling are useful for handling poorly balanced and unpredictable workloads.

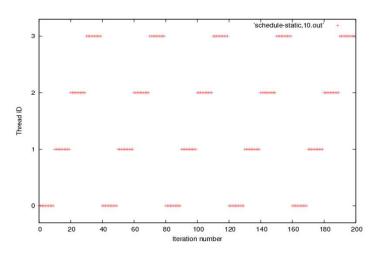


## **OpenMP Scheduling of simple for loops**

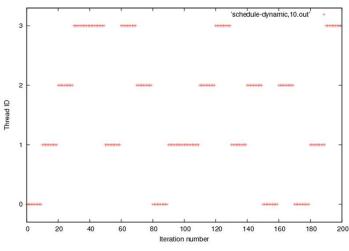




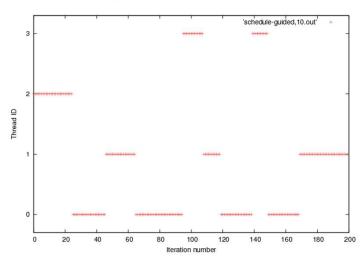
OMP\_SCHEDULE=static



OMP\_SCHEDULE=static,10



OMP\_SCHEDULE=dynamic,10



OMP\_SCHEDULE=guided,10



## 4. Deferred scheduling



#### Decided at run time:

```
Fortran auto
!$OMP do schedule( runtime )
```

- auto (automatic scheduling)
  - programmer gives implementation the freedom to use any possible mapping.
- runtime
  - schedule is one of the above or the previous two slides
  - determine by either setting OMP\_SCHEDULE, and/or calling omp\_set\_schedule() (overrides env. setting)
  - find which is active by calling omp\_get\_schedule()

#### Examples:

- environment setting:
   export OMP\_SCHEDULE='guided'
   export OMP\_NUM\_THREADS=4
   ./myprog.exe
- call to API routine:



## Final remarks on scheduling



- Please check your compiler documentation for implementationdependent aspects
- An implementation may add its own scheduling algorithms
  - code using specific scheduling may be at a disadvantage
  - recommendation: Allow changing of schedule during execution
- If runtime scheduling is chosen and OMP\_SCHEDULE is not set
  - execution starts with implementation-defined setting



## **Collapsing loop nests**



#### Example: Two nested loops

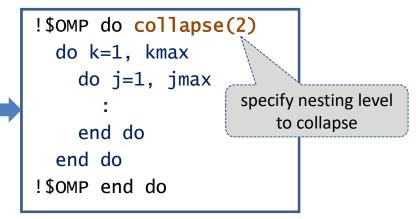
```
!$OMP do Fortran
do k=1, kmax
do j=1, jmax
:
end do
end do
!$OMP end do
```

- assume kmax is 2, and jmax is 3
- then the workshared loop will scale to at most 2 threads

#### Therapy:

- use a collapse clause to improve scaling
- this flattens two (or more) loop nests into a single iteration space

#### Improved example:



 slicing is performed on the virtual index I<sub>coll</sub>:

I <sub>coll</sub>	0	1	2	3	4	5	sequenced by
J	1	2	3	1	2	3	serial execution
K	1	1	1	2	2	2	order

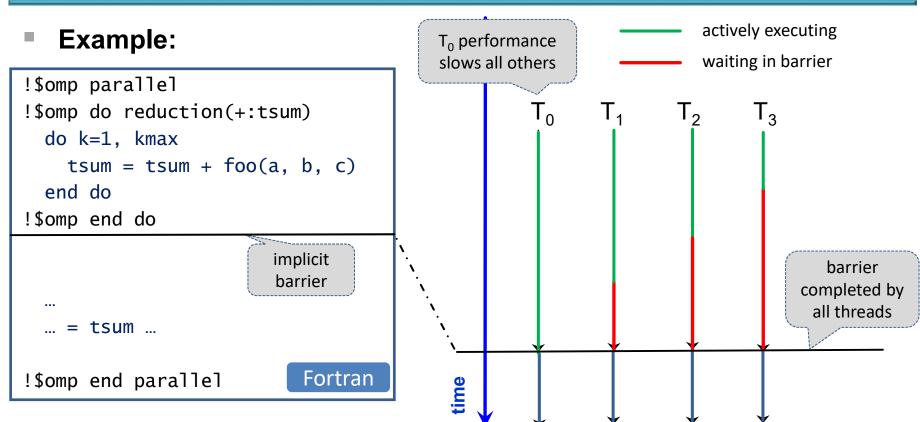
#### Restrictions:

- rectangular iteration space
- CYCLE/continue in innermost loop only



# Collecting load imbalances at synchronization points



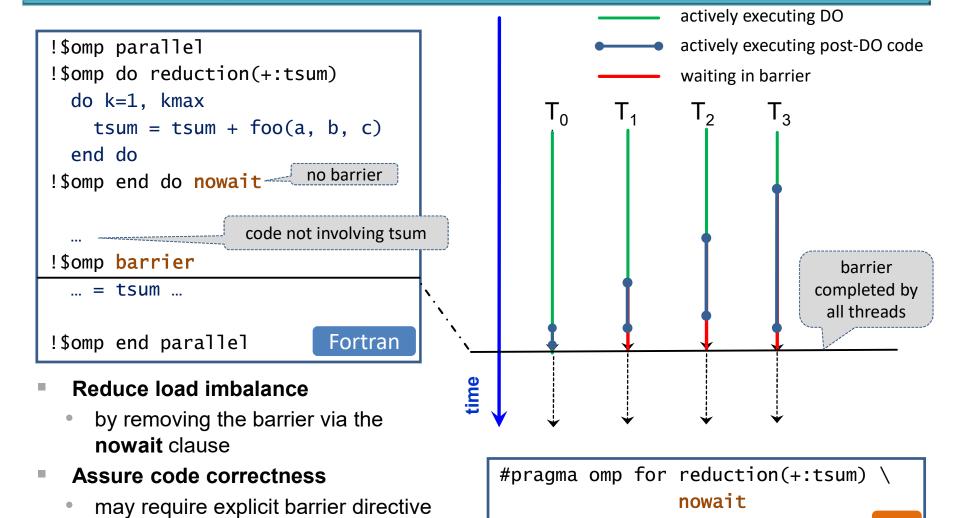


- Assumptions on code following the synchronization point:
  - does not involve tsum
  - has a load imbalance that is inverse to that of preceding code block



## nowait clause and explicit barrier directive





before tsum (or other modified

shared variable) is accessed

{ ... }

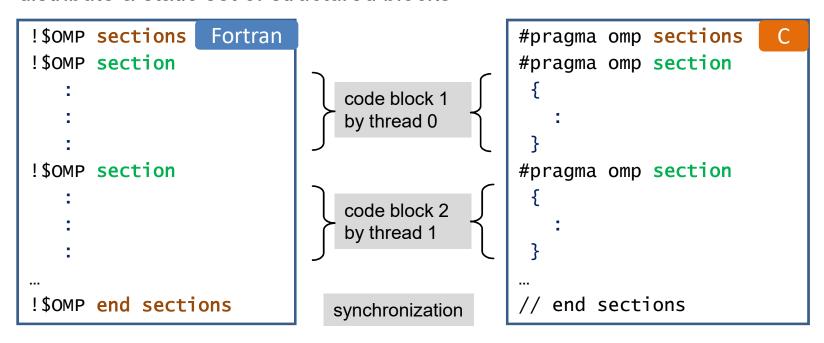


#### **Parallel sections**



#### Non-iterative work-sharing construct

distribute a static set of structured blocks



- each block is executed exactly once by one of the threads in the team
- Allowed clauses on sections:
  - private, first/lastprivate, reduction, nowait



#### Parallel sections cont'd



#### Restrictions:

- section directive must be within lexical scope of sections directive, and directly enclosed (no interleaved language construct is permitted)
- sections directive binds to innermost enclosing parallel region

   → only the threads executing the binding parallel region participate in the
   execution of the section blocks and the implicit barrier (if not eliminated with
   nowait)

#### Scheduling to threads

- implementation-dependent
- if there are more threads than code blocks, excess threads wait at synchronization point

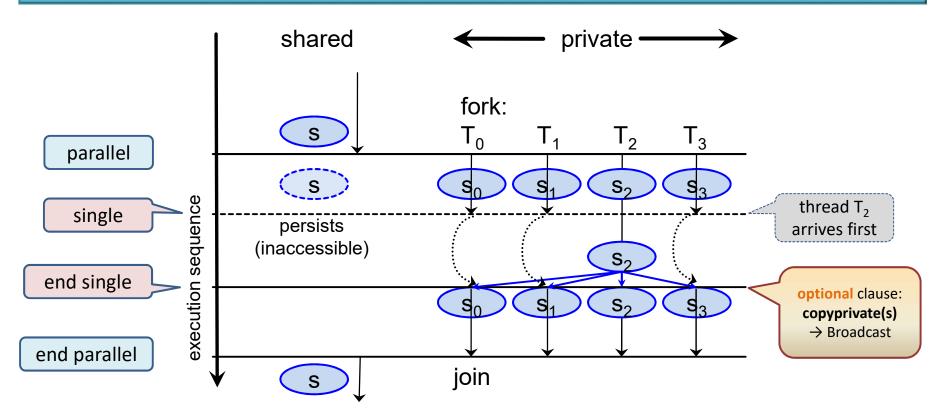
#### In modern OpenMP,

 tasking provides a much more flexible and scalable way to implement this and much more general patterns → will be treated tomorrow



## single directive and copyprivate clause





#### Execution:

- only one thread of the team executes the statements in the block
- others go to the end of the block

#### Synchronization

 of all threads at end of single block



## single directive syntax



```
float s;
real :: s
                       Fortran
                                               S = ...;
                                             #pragma omp parallel private(s)
  S = ...
!$omp parallel private(s)
                                             #pragma omp single \
!$omp single
                                                      copyprivate(s)
                            block executed by
                            one thread only
!$omp end single &
                                                  // end single
!$omp
       copyprivate(s)
 ... = ... + S
!$omp end parallel
                                               // end parallel
```

#### Note:

 update of shared variables inside a single block is safe against subsequent accesses, due to synchronization at the end of that block

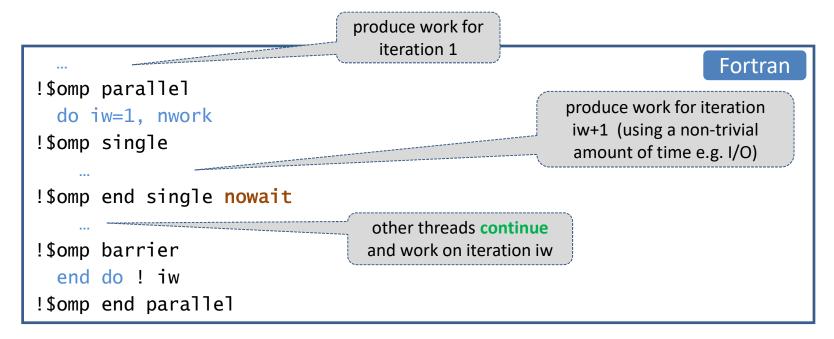


## Work sharing with single: the nowait clause



#### Implement a self-written work scheduler

one possible scheme (of many), sketched only:



- not the most efficient method
  - → preferably use tasking (covered tomorrow); the single construct will be relevant in that context





# Global variables and threading



## Global variables and their default scope



#### Examples:

```
module my_globals Fortran
  implicit none
  integer :: my_count
  real, allocatable :: a(:)
  ...
end module
```

```
REAL :: A(1000) FORTRAN 77
INTEGER :: MY_COUNT

COMMON / MY_GLOBS / A, MY_COUNT

#define NMAX 1000
float a[NMAX];
void my_func() {
  extern float a;
  ...
}
```

- Such variables by default have shared scope
- The same applies for variables with the SAVE (Fortran) or static (C) attribute

## Implication:

 code using such memory is often not thread-safe, unless mutual exclusion mechanisms are used when accessing the objects



## Privatizing global objects



- When program semantics requires that each thread work on its own copy, privatization is necessary
  - not exactly the same as private variables → separate syntax needed
- **C**:
  - #pragma omp threadprivate(list)
  - list is a comma-separated list of file-scope, namespace-scope, or static block-scope variables that do not have incomplete types
- Fortran:
  - !\$omp threadprivate(list)

directive placed in declaring program unit

- list is a comma-separated list of named variables and named common blocks. Common block names must appear between slashes.
- Objects start out with master copy existing only
  - thread-private copies (with undefined values) spring into existence when the first parallel region is started



## **Further properties of threadprivate storage**



#### Copyin clause

- broadcasts object values from master copy to threadindividual copies
- works analogous to the firstprivate clause

```
allocate( a(ndim) )
    a(:) = ...
!$omp parallel copyin(a)
    ... = a(i) + ... uses value set on
    a(i) = ...
!$omp end parallel
```

#### Subsequent parallel regions:

- thread-individual copies retain their values (by thread) if
- second parallel region not nested inside first
- same number of threads is used
- 3. no dynamic threading is used

**Note:** none of the potential violations of the above three rules are dealt with in this course

#### **Recommendations:**

- Avoid using global variables in the context of threading
- Use object-based design instead





## ... useful varia



#### The master construct



```
!$omp master

block
!$omp end master
```

```
#pragma omp master
{ block }
```

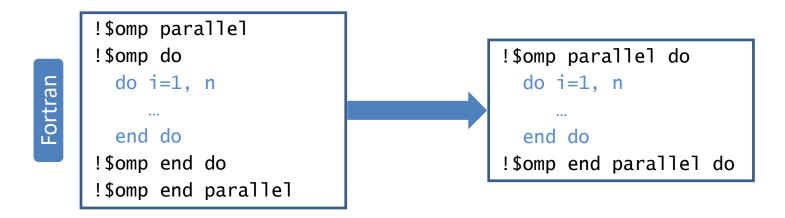
- Only thread zero (from the current team) executes the enclosed code block
  - there is no implied barrier either on entry to, or exit from, the master construct. Other threads continue without synchronization
- Notes:
  - Not all threads must reach the construct; if the master thread does not reach
    it, it will not be executed at all
  - this is not a work sharing construct, it only serves for execution control



#### **Combined constructs**



- Certain combinations of constructs can be fused
  - the result is a single construct that behaves as if the two individual ones were tightly nested
  - may be more efficient due to reduced synchronization needs
  - is often easier to read
- **Example: joint "parallel do"** (C has "parallel for" here ...)



both variants have the same semantics.



## **Conditional parallelism**



Put an "if" clause on a parallel region

```
!$omp parallel if (n > 8000)

!$omp end parallel process work item of size O(np)
```

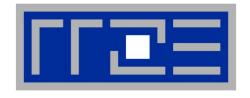
- specify a scalar logical argument
- may require manual tuning for properly dealing with thread count dependency etc.

#### Specific uses:

- execute serially for small problem sizes (parallel overhead may reduce performance)
- 2. suppress nested parallelism in a library routine:

Now: Third exercise session





# OpenMP 4.0 SIMD (vectorization) directives

# Optimization of innermost loop structures

Acknowledgment is due to M. Klemm (Intel)

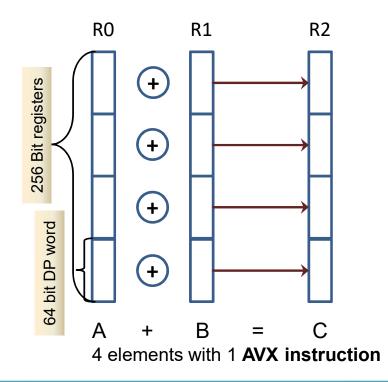


## SIMD - single instruction multiple data



#### Example:

- Sandy Bridge vector unit
- 256 Bit SIMD
- addition of 8 Byte words



#### Instruction capability

 1 vector add and 1 vector mult per cycle → theoretical Peak 8 Flops/cycle (double precision)

### LD/ST issue capability for Sandy Bridge

- 4 Words LD/cycle
- 4 Words ST/(2 cycles)
- performance boost depends on algorithm, including its temporal locality properties

#### More recent processors may have more advanced units

- more SIMD lanes
- additional vector operations



## Before OpenMP 4.0 ...



- material in the programmers had to rely on auto-vectorization,
  - or use non-portable extensions
    - > programming models (e.g. Intel Cilk Plus)
    - intrinsics (e.g. \_mm\_add\_pd())
    - > compiler pragmas

```
#pragma omp parallel for
#pragma vector always
#pragma ivdep
for (int i=0; i<N; i++) {
   a[i] = b[i] + ...;
}</pre>
```

which may or may not get ignored by the compiler



## **OpenMP SIMD loop construct**



#### Vectorize a loop nest

- cut into chunks that fit into a SIMD vector register
- without parallelization of the loop body

#### Syntax

```
#pragma omp simd [clause[[,] clause], ...]
for loops
```

```
!$omp simd [clause[[,] clause], ...]
do loops
[!$omp end simd] Fortran
```



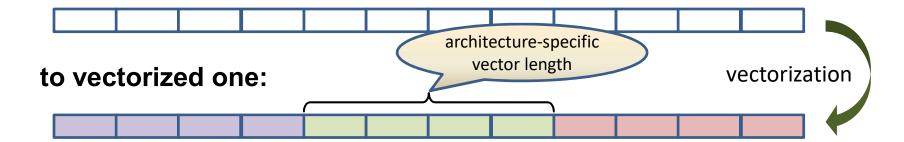
## Simple example



#### Scalar product

```
void sprod(float *a, float *b, int n) {
  float sum = 0.0f;
#pragma omp simd reduction(+:sum)
  for (int k=0; k<n; k++) {
    sum += a[k] * b[k];
  }</pre>
```

#### Converts serial element-wise execution





## **Data Sharing Clauses**



- Existing ones adapted to SIMD-style execution
  - required for more complex loop bodies
- private (var-7ist)
   create uninitialized vectors for variables in var-list
   (loop iteration variables are private by default)
- lastprivate (var-list)
  copy last iteration value to variable at the end of the construct
- reduction (op:var-list)
  create private copies for variables in var-list and apply the reduction operation op at the end of the construct





## Loop clauses (1)



- safelen (length)
  - maximum distance between iterations that can run concurrently without breaking any dependencies

```
#pragma omp simd safelen(5)
  for (int k=j; k<n; k++) {
    b[k] = a[k] * b[k-j];
}</pre>
```

- programmer assures j > 5
- compiler can use a vector length of at most 6
- linear (list[:linear-step])
  - produce private copy of a variable that is in linear relationship with the loop iteration variable:  $x_i = x_{start} + (i i_{start}) * linear-step$



## Loop clauses (2)



- aligned (list[:alignment])
  - specifies that variables in the list are aligned, either by the specified integer value of alignment in units of bytes, or in implementationspecific manner
- collapse(n)
  - collapse iteration space of a SIMD loop nest



# **SIMD** worksharing construct



### Parallelize and vectorize a loop nest

- distribute iteration space of loops across threads
- subdivide loop chunks to be processed in SIMD registers

#### Syntax



```
#pragma omp for simd [clause[[,] clause], ...]
for loops
```

Fortran

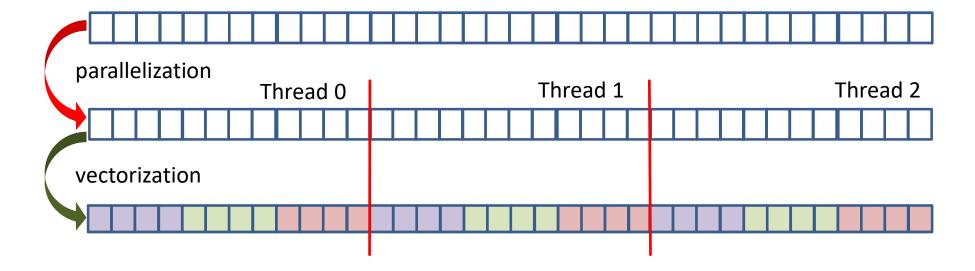
```
!$omp do simd [clause[[,] clause], ...]
do loops
[!$omp end do simd]
```



# Scalar product again ...



```
void sprod(float *a, float *b, int n) {
  float sum = 0.0f;
#pragma omp for simd reduction(+:sum)
  for (int k=0; k<n; k++) {
    sum += a[k] * b[k];
  }
</pre>
assume invocation by
all threads executing in a
parallel region
```





#### **Function vectorization**



#### Function call inside SIMD region

```
float min(float a, float b) {
  return a < b ? a : b;</pre>
float distsq(float x, float y) {
  return (x - y)*(x - y);
                   may fail if functions
                    outside file scope
void example()
#pragma omp for simd
  for (i=0; i<N; i++) {
    d[i] = min(
      distsq( a[i],b[i] ),c[i] );
```

- Therapy: explicitly declare for use in vectorized loops
  - C/C++ syntax

```
#pragma omp declare simd
function def. or decl.
```

Fortran syntax

```
!$omp declare simd &
!$omp (proc-name-list)
```

- clauses are also supported
- causes generation of multiversion code by the compiler



# **Code generation for SIMD functions**



#### vectorized versions of generated functions are shown

```
#pragma omp declare simd
                                        vec8 min_v(vec8 a, vec8 b) {
float min(float a, float b) {
                                           return a < b ? a : b;
  return a < b ? a : b;
#pragma omp declare simd
                                       vec8 distsq_v(vec8 x, vec8 y) {
float distsq(float x, float y) {
                                         return (x - y)*(x - y);
  return (x - y)*(x - y);
                                       }
                                            no SIMD directives permitted
void example() {
                                            inside vectorized functions!
#pragma omp for simd
  for (i=0; i<N; i++) {
    d[i] = min(
      distsq( a[i],b[i] ),c[i] );
                                        vd = min_v(
                                              distsq_v (va, vb), vc );
```



# Clauses applicable for declare simd



- simdlen (length)
  generate function to support supplied vector length
- uniform (argument-list)
  argument has a constant value between iterations of invoking loop
- inbranch vs. notinbranch function always / never called from inside an if statement
- linear (list[:linear-step])aligned (list[:alignment])reduction (op:var-list)



#### Final remarks on SIMD



#### Case studies on vectorizable applications:

- show performance improvements of factor 1.5 4.3 compared to auto-vectorized code
- you may not be as successful, but a 20% performance improvement for 45 min optimization work is also quite nice

#### Resolution of dependencies

may sometimes involve code restructuring and splitting of loops

# Further features available: combination of device control directives with SIMD

- platform dependence
- not discussed in this talk

Now: Fourth exercise session





# More on Synchronization and Correctness

Memory model
Identifying correctness problems
Named critical regions
Atomic operations
Loop dependencies
Mutual exclusion with locks



# **Concurrent updates on shared variables**



#### Scenario:

```
real :: a

fix number of threads
for parallel execution

a = 0

!$omp parallel shared(a) num_threads(2)

a = a + 1

write(*,'(''a on thread ',i0,' is ',i0)') &

omp_get_thread_num(), a

!$omp end parallel

write(*,'(''a after construct is ',i0)') a
```

possible results in first write

Thread 0	Thread 1
1	1
2	1
1	2

possible results in second write: 1 or 2

- the above is non-conforming
- data race causes unpredictable results to be produced

#### Reason:

- different threads can have different views on same variable: temporary view (in-register value) vs. memory value
- these two views become inconsistent when a thread modifies the variable



# **Memory consistency rules**



#### Flush Operation

- is performed on a set of (shared) variables or on the whole threadvisible data state of a program
- discards temporary view:
  - → modified values are forced to cache/memory (requires exclusive ownership)
  - → next read access must be from cache/memory
- further memory operations only allowed after all involved threads complete flush:
  - → restrictions on memory instruction reordering (by compiler)

!\$omp flush [list]

recommend to **avoid** use of explicit flushes

# Ensure consistent view of memory:

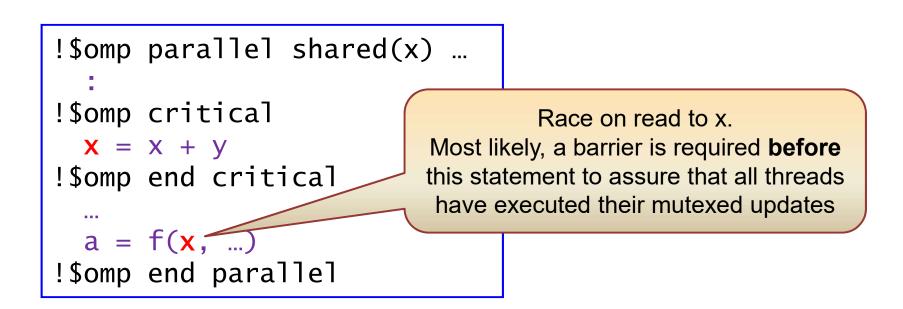
- Assumption: want to write a data item with one thread, read it with another one
- Order of execution required:
- 1. thread 0 writes to shared variable
- 2. thread 0 flushes variable
- 3. thread 1 flushes same variable
- 4. thread 1 reads variable
- The challenge is to assure step 3 happens after step 2
- OpenMP construct synchronization semantics assure this as well as the necessary implicit flush operations (if correctly used)



# But it is possible to make mistakes ...



- Example: update via critical region
  - mutual exclusion is only assured for the statements inside the block i.e., subsequent threads executing the block are synchronized against each other
- If other statements access the shared variable, you may be in trouble:





# Using Intel Inspector on x86-based systems



#### OpenMP correctness analysis:

- no special compiler option needed (except perhaps –g)
- GUI also for Linux-based system
- Identify memory issues in addition to threading issues
  - leaks, dangling pointers etc.
- Start up GUI
  - prerequisites: set up environment and possibly stack limit
  - then, invoke the GUI with inspxe-gui &
  - command line inspxe-cl is also available, but will not be discussed in this talk



# Starting up the GUI → start a new project

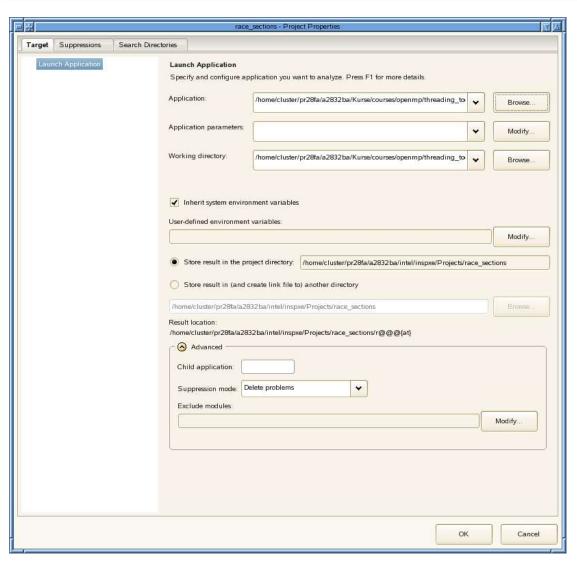


<u>F</u> ile View Help		
Welcome 🕱		·
Project name:	Race_1  • O	enter project name then pross greate project"
Location:	/home/hpc/pr28fa/a2832ba/intel/inspxe/projects	then press "create project"
	Create Project	Cancel
	Current project: heat_tune1  Threading Error Analysis / Detect Deadlocks and Data Races	№ Project
	Threading Error Analysis / Locate Deadlocks and Data Races  Memory Error Analysis / Detect Leaks  Memory Error Analysis / Locate Memory Problems  New Analysis	Open Project
	Recent Projects:	Recent Results:
	> tasked_integral_c > tasked_integral > demo_kurs > fp	> r004ti3 [heat_tune1] > r003ti3 [heat_tune1] > r002ti3 [heat_tune1] > r001ti3 [heat_tune1] > r000ti3 [heat_tune1]
	Introduction	n to OpenMP 84



# **Configure the project**





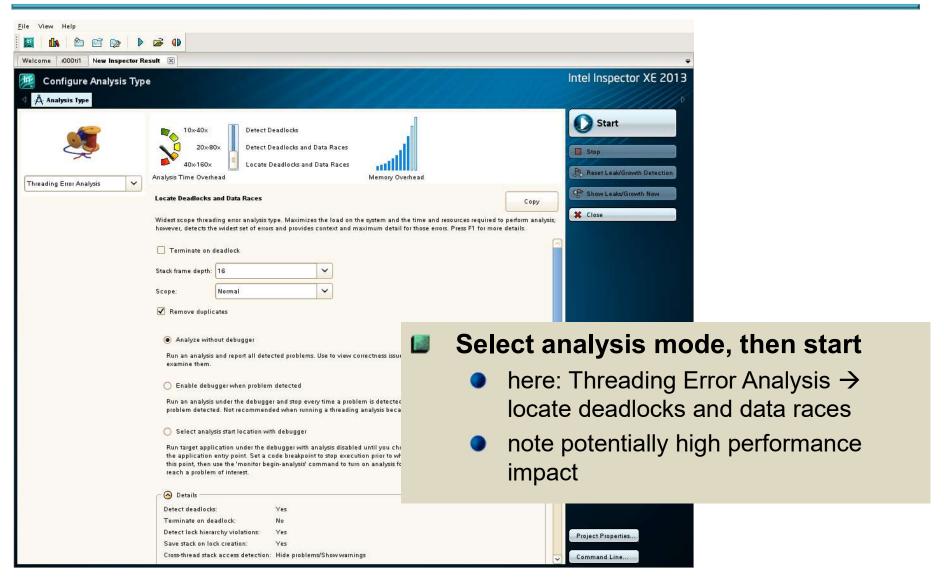
#### Needed information:

- executable name (must have been built with OpenMP)
- executable path (autocompleted)
- arguments if needed by executable
- Further advanced settings are possible



# Run Analysis: New → Analysis Result

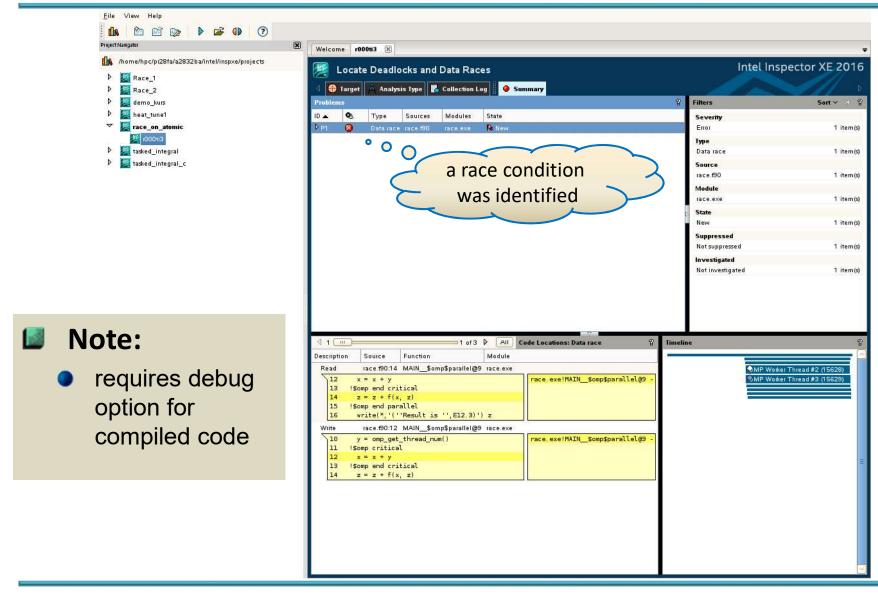






# **Error indication by severity**

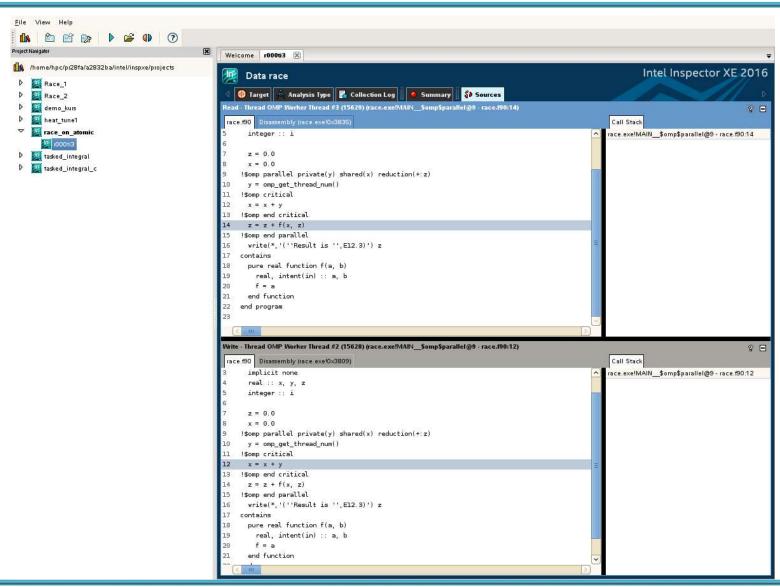






# Source window: conflicting reads/writes







# **Critical regions: consider multiple updates**



a) same shared variable

thread 0

thread 1

Fortran

```
subroutine foo()
!$omp critical
  x = x + y
!$omp end critical
```

```
subroutine bar()
!$omp critical
  x = x + z
!$omp end critical
```

critical region is **global** → OK

b) different shared variables

Fortran

```
subroutine foo()
!$omp critical
  x = x + y
!$omp end critical
```

```
subroutine bar()
!$omp critical
  w = w + z
!$omp end critical
```

mutual exclusion not required → unnecessary loss of performance



# Named critical regions



#### Solution:

use a named critical

Fortran

```
subroutine foo()
!$omp critical (foo_x)
  x = x + y
!$omp end critical (foo_x)
```

```
subroutine bar()
!$omp critical (foo_w)
  w = w + z
!$omp end critical (foo_w)
```

mutual exclusion only if same name is used for critical regions acting on different code blocks

- Note: The atomic directive is bound to the updated variable
  - → problem does not occur when such a directive is used.



# More variants of atomic operations



#### Assumption:

- v, w private or shared scalar variables
- x a shared scalar variable

#### Atomic read:

```
#pragma omp atomic read
v = x;
```

#### Atomic write:

```
#pragma omp atomic write
x = v;
```

#### Atomic capture

```
!$omp atomic capture
v = x
x = x <op> w
!$omp end atomic
```

 different ordering of statements also allowed

#### Not atomic:

 evaluation of expressions or updates on v

# Atomic update:

- !\$omp atomic update
- same as "traditional" atomic directive



# **Atomic operations require care**



#### Atomic directives

 permit the programmer to explicitly program with race conditions

#### Rationale for use:

- performance
- tailored synchronizations → will usually require explicit flush operations (not discussed)

# A Programmer's responsibility

- to assure that no inconsistencies result → must evaluate results from all possible interleavings of execution by different threads
- tools might not be able to observe problems

### Synchronization effect

- apart from the value change on the variable itself being visible, no synchronization is done
- sequentially consistent atomic operations:

perform a flush on all threadvisible variables (but no synchronization otherwise). Semantics are the same as for such operations in the C++11 standard



# Dealing with dependencies in a loop



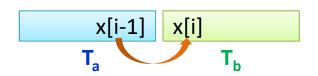
#### Variant of theoretical exercise

 race condition i-1 → i on one statement

```
real :: a(n), b(n), x(n)
a = ...; b = ...; x(1) = ...
!$omp parallel shared(a,b,x)
!$omp do
do i=2, n
b(i) = f1( a(i), b(i) )

x(i) = a(i) * x(i-1) + b(i)
a(i) = f2( b(i), x(i) )
end do
!$omp end do
!$omp end parallel Fortran
```

 race occurs on chunk boundaries executed by different threads:



#### Ordered clause and directive

Syntax: uses a clause for the loop and an ordered region inside the loop body

```
!$omp do ordered
do ...
!$omp ordered
...
!$omp end ordered
...
end do
!$omp end do
Fortran
```

- statements in ordered region are executed in same order as the loop's iteration variable is increased in a serial execution
- statements outside the ordered region can execute in parallel
- only one ordered region permitted



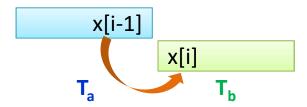
# **Corrected example**



Assures that code block with flow dependency is effectively serialized

```
!$omp parallel shared(a,b,x)
!$omp do ordered
do i=2, n
  b(i) = f1( a(i), b(i) )
!$omp ordered
  x(i) = a(i) * x(i-1) + b(i)
!$omp end ordered
  a(i) = f2( b(i), x(i) )
end do
!$omp end do
!$omp end parallel
Fortran
```

•  $T_a$  signals completion of its chunk to  $T_b \rightarrow$  synchronization avoids the race





# **Explicit cross-iteration dependency specification**

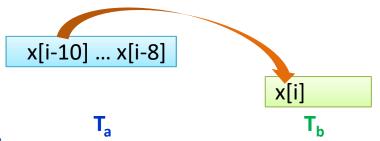


#### depend clause

```
#pragma omp for ordered (1)
for (i=10; i<N; i++) {
  ... // independent execution
#pragma omp ordered \
                              consumer T<sub>h</sub>
                              must wait
    depend(sink:i-10) ~
  x[i] = a[i] * x[i-10] + b[i];
#pragma omp ordered \
                           supplier T<sub>a</sub> signals
                              completion
    depend(source)
    // independent execution
```

#### Additional semantics:

- may be needed due to possibly different (schedule dependent) chunk assignment
- might improve concurrency





#### **Doacross loop nests**



#### Ordered clause with a nesting depth specification

```
#pragma omp for ordered (2)
    dependencies span across
    two nested loops

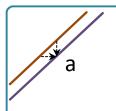
for (i=1; i<N; i++) {
    for (j=1; j<N; j++) {
    #pragma omp ordered depend(sink:i-1,j) depend(sink:i,j-1)
        a[i][j] = ... * a[i-1][j] + ... * a[i][j-1];

#pragma omp ordered depend(source)
    }
}</pre>
```

- parallel execution within diagonal i+j=d is possible, in order of d
- loop schedule tuning will be required



beware potential deadlocks (incorrectly specified dependencies)

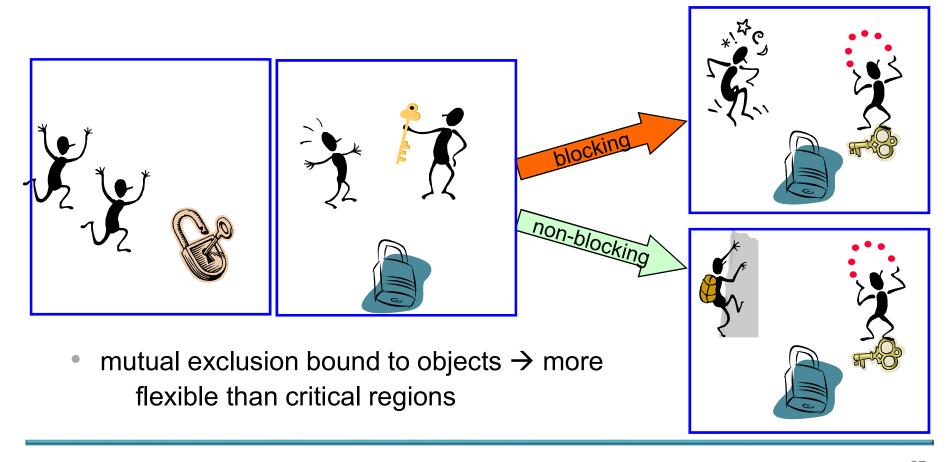




### **Mutual exclusion with locks**



# A shared lock variable can be used to implement specifically designed synchronization mechanisms





# **OpenMP lock variables**



- Two variants of locks exist:
  - simple locks
  - nestable locks (will not be dealt with in detail in this course)
- Declaration of a lock variable



# **Preparing locks for use**



- The initial state of a lock variable is "uninitialized"
  - i.e. it is not actually associated with a lock variable
- Need to invoke an initialization function on it before it is used
  - subroutines / void functions provided in OpenMP run time

Name	Purpose
<pre>omp_init_lock(omp_lock_t *lock)</pre>	initializes an uninitialized lock; the lock variable has the state "unlocked" on return
<pre>omp_destroy_lock(omp_lock_t *lock)</pre>	destroys a lock that has the state "unlocked".
<pre>omp_init_nest_lock           (omp_nest_lock_t *lock)</pre>	initializes an uninitialized nestable lock; the lock variable has the state "unlocked" on return, and its nesting count is zero.
<pre>omp_destroy_nest_lock       (omp_nest_lock_t *lock)</pre>	destroys a nested lock that has the state "unlocked".

Fortran: replace \*lock argument by integer of appropriate kind



# Lock ownership



- An initialized OpenMP lock can be in one of the states unlocked, or locked
- The (unique) task region that has successfully acquired the lock is said to own the lock
  thread + context it is executing in
- Only the task region that owns the lock can release it, returning it to the unlocked stage.

Name	Purpose
<pre>omp_set_lock(omp_lock_t *lock)</pre>	If the lock is already locked by another task region, block until the state of the lock changes. If the lock is in the state unlocked, acquire it, setting it to the locked state, and continue execution.
<pre>omp_unset_lock(omp_lock_t *lock)</pre>	Release the lock that is owned by the executing task region.

#### Notes:

- state combinations not described in the table are not permitted (e.g., a task region trying to unset a lock it does not own)
- the lock variable must be shared in the calling scope



# Simplest possible example



### Usage pattern analogous to named critical region

 programmer is responsible for relationship between lock and objects protected by it

```
#include <omp.h>
use omp_lib
                             Fortran
integer(omp_lock_kind) :: lock
                                         omp_lock_t lock;
                                         omp_init_lock(&lock);
call omp_init_lock(lock)
                      starts in unlocked state
                                         #pragma omp parallel
!$omp parallel
                                              omp_set_lock(&lock);
call omp_set_lock(lock)
                               only one thread at a
                                time gets to play
                                with the red balls
                                              omp_unset_lock(&lock);
call omp_unset_lock(lock)
                               release resources
!$omp end parallel
call omp_destroy_lock(lock)
                                         omp_destroy_lock(&lock);
```



# Non-blocking attempt at ownership



#### Function call signature

- if the lock is already locked by another task region, return "false"
- if the lock has the state unlocked, acquire it (setting the state to locked) and return the value "true".

#### Permits implementing additional concurrency



# Final notes on locking



#### Potential performance issues

- locks are a relatively expensive synchronization mechanism
- lock contention (algorithm dependent)

#### Programming issues

easy to produce deadlock (non-composable against other constructs)

#### Nestable locks

extended semantics for repeated locking (additional nesting count)

### Locks with hints (OpenMP 4.5)

- programmer can specify expected usage pattern, but the actual effect is implementation dependent
- this is an advanced topic, and using this feature may require special hardware features (transactional processing)
- OpenMP 5.0 will likely have some changes in this area



# Synchronization overhead



## Syncbench from the EPCC OpenMP microbenchmarks is used

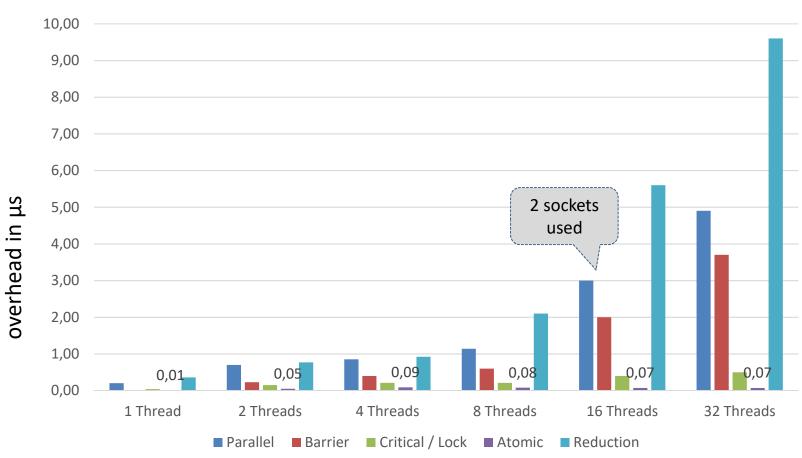
- evaluates the overheads for all synchronizing constructs systematically
- overhead is what remains even if no workload is processed
- Showing results as a function of thread count
  - alternatively, depending on node architecture and used compiler
- Note order of magnitude
  - a microsecond typically corresponds to a couple of thousand CPU cycles



# **Thread count dependence**



#### Westmere 4-socket node overhead with ICC 15

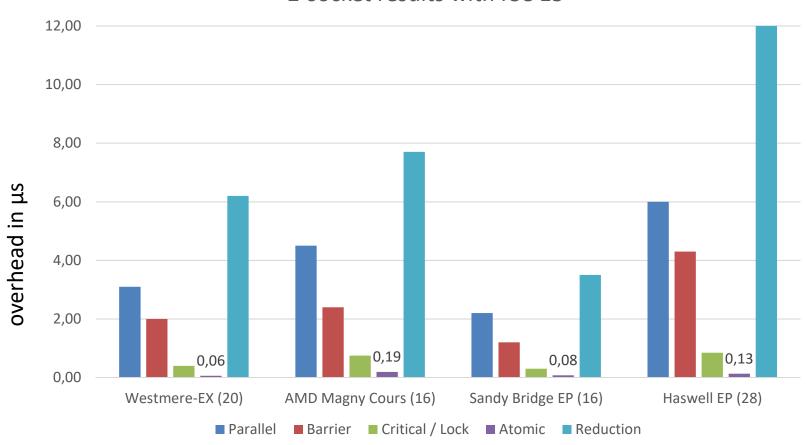




# **Architecture dependence**



#### 2-socket results with ICC 15

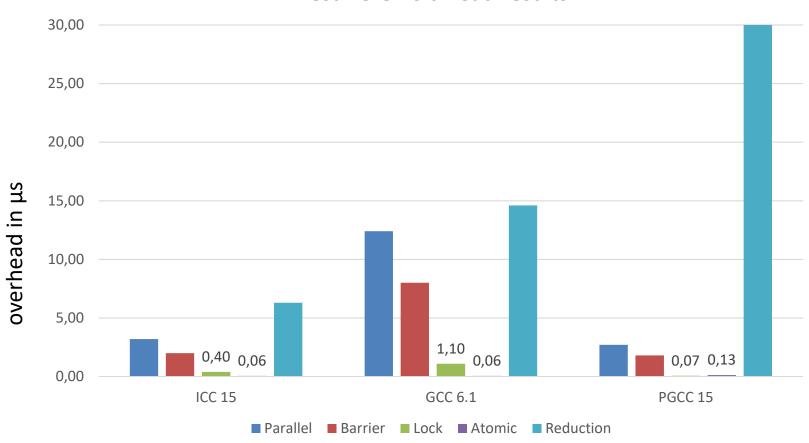




# **Compiler dependence**



#### Westmere 20 thread results





# How to deal with synchronization overhead



#### Therapy 1:

- use the right compiler
- note: x86 does not (yet) support hardware synchronization

#### Therapy 2:

- execute serially for small problem sizes
- conclude parallel execution if not needed any more

### Therapy 3 (may be most effective):

- reduce the synchronization requirements of your algorithm
- Examples: nowait clause, or extend parallel regions to reduce number of forks/joins

Now: Fifth exercise session





# **Tasking**

Work sharing for irregular problems, recursive problems and information structures

Acknowledgement due to L. Meadows/T. Mattson (Intel) for their SC08 slides



## **Processing information structures**



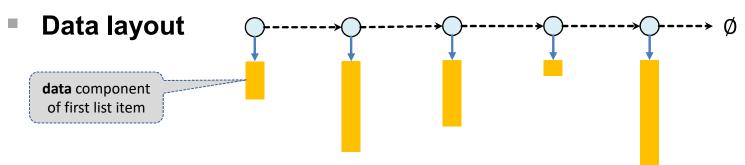
Example: linked list

Fortran

C

```
type :: list
  type(list), pointer :: next => null()
  real, allocatable :: data(:)
end type
```

```
typedef struct {
  List *next;
  real *data; int n;
} List;
```



- each list item may carry a different payload
- parallel processing on a per-list-item basis → load imbalance is likely to occur
- the list as a whole is intended to be shared (i.e. no copies of payload should be created during processing)



# Serial processing of a linked list



```
subroutine process_list(head)
  type(list), target :: head
  type(list), pointer :: p

p => head
  do while (associated(p))
    call do_work(p%data)
  p => p%next
  end do
end subroutine Fortran
```

```
void process_list(list *head) {
  list *p = head;

while (p) {
    do_work(p->data, p->n);
    p = p->next;
}
```

#### Not a regular loop in the sense of OpenMP

 cannot use work sharing constructs even though potential concurrency is obvious.

#### In general:

API calls for processing information structures often are recursively invoked
 → OpenMP 2.5 offers no means of parallelization for this situation, although
 concurrency can be formally exposed.



#### What is a task?



#### Aim: make OpenMP worksharing more flexible

#### Semantics:

- When a thread encounters a task construct, a task is generated from the code of the associated structured block.
- Data environment of the task is created (according to the data-sharing attributes, defaults, ...)
- The encountering thread may immediately execute the task, or defer its execution.
  - In the latter case, any thread in the team may be assigned the task.

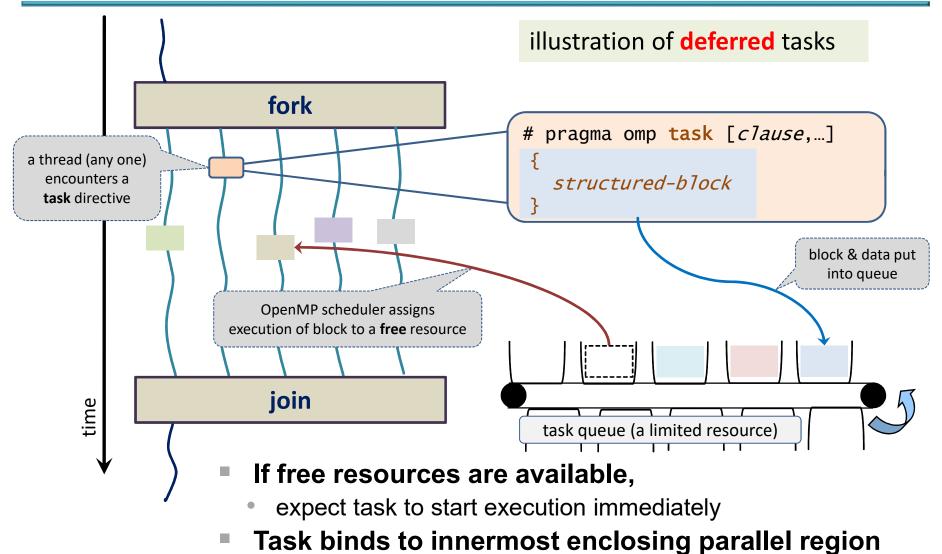
#### Introduced with OpenMP 3.0

additional features and improvements added in later versions of the standard



# **Concept of tasking**







# Simplest example: code sections



```
program code_sections
                              Fortran
 use mod functions
                                             int main() {
 implicit none
                                               float a, b;
 real :: a, b
                                               int n = ...;
                                             #pragma omp parallel
 integer :: n = ...
                                                                        only thread 0
!$omp parallel
                                             #pragma omp master
                                                                        creates tasks
!$omp master
!$omp task
                                             #pragma omp task
   a = function_1(n)
                                                { a = function_1(n); }
!$omp end task
                      concurrently executed
                                                                        a and b have
                       if sufficiently many
                                                                        shared scope
                        threads available
                                             #pragma omp task
!$omp task
   b = function_2(n)
                                                { b = function_2(n); }
!$omp end task
                                               } // end parallel and master
                        no synchronization
!$omp end master
                      (different than single)
!$omp end parallel
 write(*,*) a + b
                                             printf("%f\n", a + b);
                          threads waiting here
end program
                           will be put to work
```



# Data scoping in task regions



```
int main() {
  float a, b;
  int n, i;
  a = ...; n = ...;
#pragma omp parallel private(b)
  b = ...;
#pragma omp master
                         i is private
#pragma omp task
                         (loop index)
     for (i=0;i<n;i++) {
                                  b is
                              firstprivate
       ... = a + foo(i);
            a is shared (because it is
              shared in all lexically
              enclosing constructs)
         default scopings
```

#### Recommendation:

- use a default(none) clause on all task directives
- explicitly specify the scoping for each data object



#### Tasked linked list



```
subroutine process_list(head)
                                                 void process_list(list *head) {
  type(list), target :: head
                                                   list *p = head:
 type(list), pointer :: p
                                                 #pragma omp parallel
!$omp parallel
                               only one thread
                                creates tasks
!$omp single shared(p)
                                                 #pragma omp single \
  p => head
                                                              nowait shared(p)
 do while (associated(p))
!$omp task firstprivate(p)
                                                     while (p) {
    call do_work(p%data)
                                                 #pragma omp task firstprivate(p)
                                task region (includes
                               procedure execution)
                                                       { do_work(p->data, p->n); }
!$omp end task
    p => p%next
                                                       p = p->next;
  end do
                               synchronization
!$omp end single nowait
                                                   } // end single
                               here → all tasks
!$omp end parallel
                                                   // end parallel
                                   done
end subroutine
                          Fortran
```

### Need to have local pointer p firstprivate:

- avoid race condition on shared original (vs. subsequent update)
- assure that association status is copied to thread executing the task region



## The "if" clause on a task directive



- When "if" argument evaluates to "false",
  - the parent task must **suspend** execution until the encountered task region has been completed (an "undeferred task"). However, it is not fully clear from the standard whether the child task must be executed by the same thread.
  - but otherwise semantics are the same (with respect to data environment and synchronization) as for a "deferred" task

```
#pragma omp task firstprivate(p) if ( sizeof(p->data) > threshold )
      { do_work(p->data); }

!$omp task firstprivate(p) if ( size(p%data) > threshold )
      call do_work(p%data)
!$omp end task
```

- User-directed optimization ("task pruning")
  - avoid overhead for deferring small task
  - avoid creating too many tasks (resource limits!)
  - cache locality / memory affinity are likely to change



# **Recursive tasking**



#### Divide and conquer

```
float dag(float *data, int n) {
  float xl, yl;
                               private at
  int n1 = ..., n2 = ...;
                               this point
  float *data2 = ...;
  if (n1 < THRESHOLD)
                            terminate
                            recursion
      { ... }
#pragma omp task shared(x1)
  { x1 = daq(data, n1); }
#pragma omp task shared(y1)
  { y1 = daq(data2, n2); }
#pragma omp taskwait
  return xl - yl;
```

 initial function invocation in a parallel region, usually from a single thread

#### Previous example:

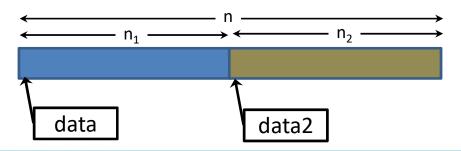
only sibling tasks are created

#### This example:

each task creates two child tasks
 → "deep hierarchy" of tasks

#### Scoping for x1, y1:

- start out as private variables
- only newly created tasks share scope with these variables
- shared scope is needed to communicate data outside the task regions



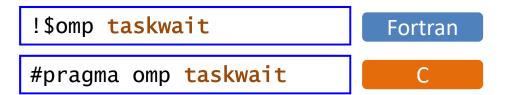


# **Tasking-specific synchronization**



#### The taskwait directive

- suspends execution until immediate child tasks of current task complete (the directive does not apply for descendants of child tasks)
- Syntax:



#### Needed in example from previous slide

- avoid race condition of assignments vs. evaluation
- avoid local variables vanishing into thin air while tasks are still executing



# Task switching



# Possible issues with task scheduling:

- large number of tasks are created → implementationdefined limit on unassigned tasks may be reached
- all currently active tasks reach a synchronization statement -> threat of deadlock?

#### Task switching

- permits a thread to suspend a task and start or resume another task at a task scheduling point
- for tied tasks, the same thread is obliged to resume execution of the suspended task later

# Task scheduling points immediately after generation of a task at the end of a task region in implicit or explicit barrier regions (wait until all tasks executed by the team are done) in a taskwait region in a taskyield region at the end of a taskgroup region

e.g., a thread that creates lots of tasks may stop doing so and start working on one of them

tasks are tied by default ..



# **Thread switching**



# pragma omp task untied

#### Default behaviour:

- a task assigned to a thread must be (eventually) completed by that thread → task is tied to the thread
- Change this via the untied clause
  - execution of task block may change
     to another thread of the team at any task scheduling point
- Deployment of untied tasks
  - Starvation scenario:

Task switching has caused the task-generating thread to run a long calculation, with the result that all generated tasks were consumed and most threads idle.

If the task that generates the work is untied, a different thread can take over the task-generating workload.



# Interactions of Untied Tasks with other OpenMP features





#### **Thread-related semantics**

used in the untied task region are likely to trip you up, for example ...

- relying on results delivered by omp\_get\_thread\_num()
  - → may become inconsistent after thread switch
- referencing and defining values stored in threadprivate global variables
  - → may access a different copy after thread switch

#### Workaround

 revert from untied to tied for the duration of problematic operations, if possible

 or use an "if (0)" clause (undeferred task might be executed by a different thread, though)



# Further potentially dangerous interactions



#### Use of threadprivate data by tied tasks

 value of threadprivate variables cannot be assumed to be unchanged across a task scheduling point. Might have been modified by another task executed by the same thread.

#### Tasks and locks:

 if a lock is held across a task scheduling point, interleaved code trying to acquire it (maybe using the same thread) may cause deadlock

**Comment:** implementation-defined task scheduling points in **untied** tasks have been removed from the standard

#### Tasks and critical regions:

 similar issue if suspension of a task happens inside a critical region and the same thread tries to access the same critical region in another scheduled task

#### Tools?

correctness tools will currently only find some of the issues that can arise



# **Programmer-defined task scheduling points**



#### Syntax and Semantics

!\$omp taskyield

Fortran

#pragma omp taskyield



 permits (but does not force) task suspension for the current task at the point where the directive is placed

#### Example

 avoid deadlock in a mutual exclusion region (taken from the OpenMP examples)

```
subroutine foo ( lock, n )
  use omp_lib
  integer(kind=omp_lock_kind) :: lock
  integer :: n
  integer :: i
  do i = 1, n
!$omp task
    call something_useful()
    do while &
       ( .not. omp_test_lock(lock) )
!$omp taskyield
    end do
    call something_critical()
    call omp_unset_lock(lock)
!$omp end task
  end do
end subroutine
                              Fortran
```



# Task group synchronization



#### Purpose:

- synchronize all tasks created inside a structured block
- includes all descendants, not only immediate child tasks

 $\leftrightarrow$  taskwait

synchronization (i.e. waiting for task completion)
 happens at the end of the taskgroup region (task scheduling point)

#### Syntax:

```
!$omp taskgroup

structured block
!$omp end taskgroup

#pragma omp taskgroup

{

structured block
}

#pragma omp taskgroup

{

structured block
}

Example:

recursive tasking with atomic

updates in each task → guarantee

completeness of updates
```

Note:



# Final and mergeable tasks



#### Final tasks

- use a final clause with a condition on a task directive
- if the condition evaluates to "true", the resulting task is always undeferred, and is immediately executed by the parent task's thread
- reduces the overhead of placing tasks in the "task pool"
- all tasks created inside task region are also final (different from an if clause)
- inside a task block,
   omp\_in\_final() can be used
   to check whether the task is final

#### Merged tasks

- using a mergeable clause may create a merged task if it is undeferred or final
- a merged task has the same data environment as its creating task region

#### Final and/or mergeable

- can be used for optimization purposes
- e.g. to optimize wind-down phase of a recursive algorithm

current implementations seem not to actively support merging.





#### Syntax

!\$omp task priority(priority\_value)

Fortran

#pragma omp task priority(priority\_value)

С

#### Semantics

- provides a hint to the run time on prioritizing (ordering) task execution
- the priority value must be a non-negative integer; higher values correspond to higher priorities; maximum value is omp\_get\_max\_task\_priority()
- do not rely on a particular ordering of tasks imposed by specifying a priority

```
#pragma omp task priority(9999)
    participants.get_coffee(100);
```



#### **Order and Chaos**



Observed output with 3 threads can be

#### Example program

```
any of ...
 s1 = ''; s2 = 'and'; s3 = 'chaos'
                                         and order chaos
                                         order chaos and
                                         chaos order and
!$omp parallel
                                         order and chaos
!$omp master
                                         chaos and order
!$omp task
                                         and chaos order
 s1 = 'order'
 write(*, fmt='(a)', advance='NO') trim(s1) // ' '
!$omp end task
!$omp task
 write(*, fmt='(a)', advance='NO') trim(s2) // ' '
!$omp end task
!$omp task
 write(*, fmt='(a)', advance='NO') trim(s3) // ' '
!$omp end task
!$omp end master
!$omp end parallel
 write(*, fmt='(a)', advance='NO') new_line('a')
```



# Introducing data-driven dependencies: the "depend" clause

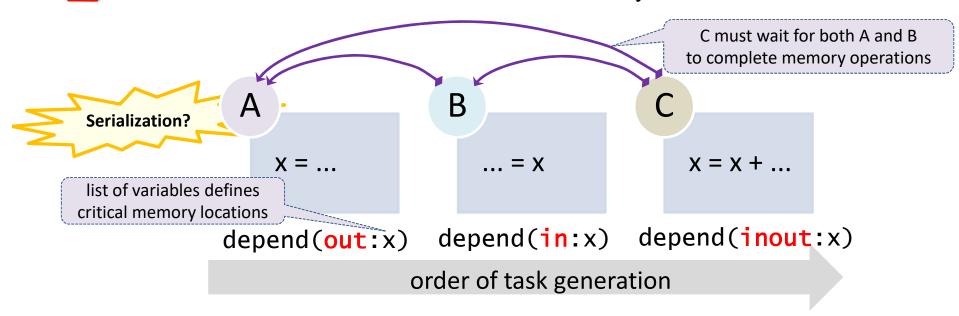


Consider

i.e., all created by the same (parent) task

a set of sibling tasks

<u> A shared variable x that is referenced or defined by more than one of them</u>



- in dependence: synchronizes memory operations against previously started tasks with an inout or out dependence on same memory location
- out or inout dependence: synchronizes memory operations against any defined dependence on same memory location for previously started task



## **Ordering the Chaos**



#### Via addition of depend clauses

```
s1 = ''; s2 = 'and'; s3 = 'chaos'
!$omp parallel
!$omp master
!$omp task depend(out:s1)
                                         avoid race conditions)
 s1 = 'order'
 write(*, fmt='(a)', advance='NO') trim(s1) // ' '
!$omp end task
!$omp task depend(in:s1) depend(out:s2)
 write(*, fmt='(a)', advance='NO') trim(s2) // ' '
!$omp end task
!$omp task depend(in:s2)
 write(*, fmt='(a)', advance='NO') trim(s3) // ' '
!$omp end task
!$omp end master
!$omp end parallel
 write(*, fmt='(a)', advance='NO') new_line('a')
```

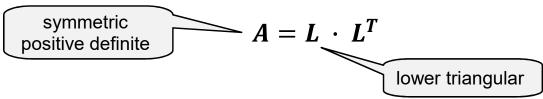
#### Observed output with 3 threads can only be order and chaos

The **type** of memory operation that is actually performed is irrelevant for the ordering properties (although it usually determines what type of dependency must be declared to

# Real-world example: Cholesky decomposition



Drawing the square root of a matrix



Recursive blocked algorithm

$A_{11}$	$A_{21}^T$		$L_{11}$	0		$L_{11}^T$	$L_{21}^T$
$A_{21}$	$A_{22}$	=	$L_{21}$	$L_{22}$	*	0	$L_{22}^T$

LAPACK algorithm ?POTRF

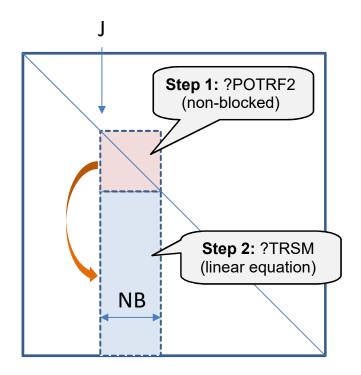


# **Loop Parallel Cholesky**



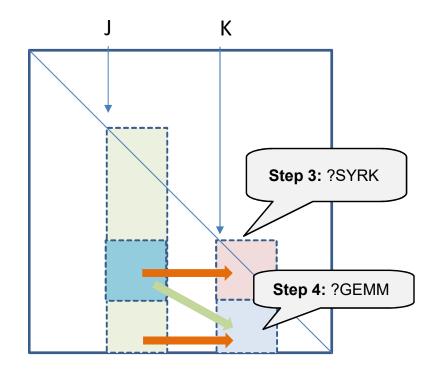
#### Phase 1

- one thread only
- "hot" block column is J



#### Phase 2

parallel updates of columns
 K = J+NB, J+2\*NB, ...



load imbalance

→ use suitable schedule



## **Loop-parallel implementation sketch**



```
!$OMP PARALLEL PRIVATE(JB, KB)
 DO J = 1, N, NB
   JB = MIN(NB, N-J+1)
!$OMP SINGLE
  Update the current diagonal block
 A(J,J), JB by JB and test for
! non-positive-definiteness
   CALL POTRF2( ... )
   IF ( J+JB.LE.N ) THEN
! using the above, solve for
! A(J+JB,J), N-J-JB+1 by JB
     CALL DTRSM( ... )
   FND TF
!$OMP END SINGLE
```

```
!$OMP DO SCHEDULE(...)
   DO K = J+NB, N, NB
     KB = MIN(NB, N-K+1)
! Update diagonal block A(K,K)
! from A(J,K)
     CALL DSYRK( ... )
     IF (K+KB.LE.N) THEN
! Update subdiagonal block A(K+KB,K)
! from A(K+KB,J) and A(K,J)
       CALL DGEMM( ... )
     END IF
   END DO
!$OMP END DO
END DO
!$OMP END PARALLEL
```

#### Reminiscence:

- Parallelization of Linear Algebra Algorithms on the KSR1, R. Bader (1994)
- same basic structure of algorithm, but OpenMP is more elegant

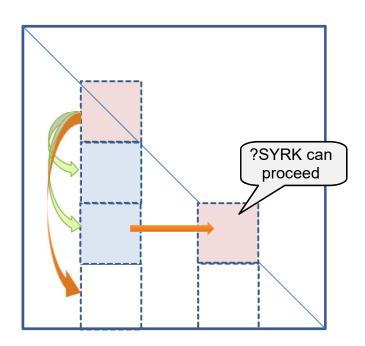


## **Extracting more parallelism**



#### Phase 1:

 multithread the TRSM update by subdividing the block column



#### Phase 2:

- multithread the GEMM update by subdividing the block column
- pipelined startup of SYRK/GEMM updates possible as phase 1 blocks complete
- Tasking makes this easy to do

#### Requirement:

need to specify the data dependencies

→ Fortran array sections in depend clauses

#### Note:

 nested parallelism has more overhead and is more difficult to manage



# **Tasked implementation sketch**



```
!$OMP PARALLEL PRIVATE(JB, JJB, KB)
 DO J = 1, N, NB
    JB = MIN(NB, N-J+1)
!$OMP SINGLE
!$OMP TASK &
!$OMP& DEPEND(inout: &
!\$OMP\& A(J:J+JB-1,J:J+JB-1))
    CALL POTRF2( ... )
!$OMP END TASK
    DO JJ = J+JB, N, NB
       JJB = MIN(NB, N-JJ+1)
!$OMP TASK &
!$OMP& DEPEND(in: &
!\$OMP\& A(J:J+JB-1,J:J+JB-1)) \&
!$OMP& DEPEND(inout: &
!\$OMP\& A(JJ:JJ+JJB-1,J:J+JB-1))
      CALL DTRSM( ... )
!$OMP END TASK
                         explicit
    END DO
                      synchronization
                      point removed
```

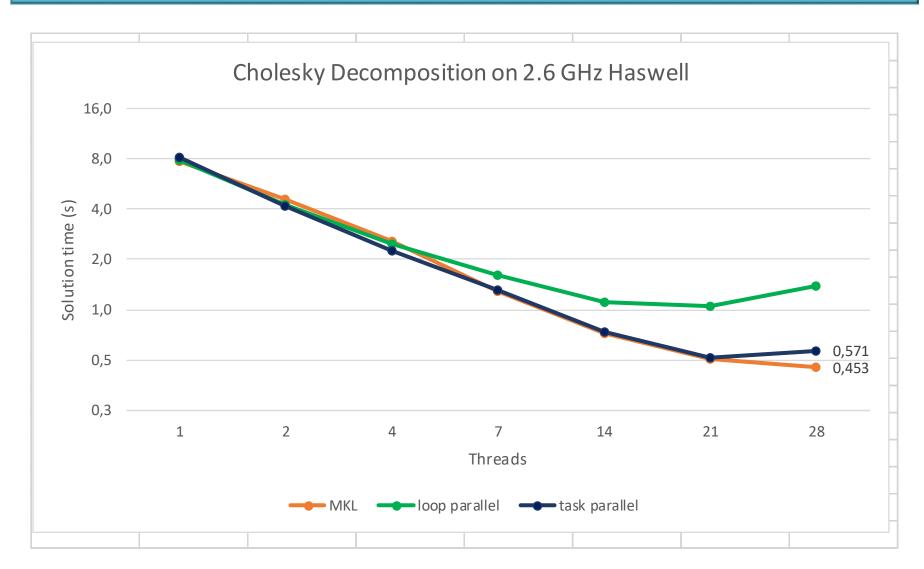
```
DO K = J+NB, N, NB
    KB = MIN(NB, N-K+1)
!$OMP TASK DEPEND(in: &
!\$OMP\& A(K:K+KB-1,J:J+JB-1))
!$OMP& DEPEND(inout: &
!\$OMP\& A(K:K+KB-1,K:K+KB-1))
    CALL DSYRK( ... )
!$OMP END TASK
    DO JJ = K+KB, N, NB
         JJB = MIN(NB, N-JJ+1)
!$OMP TASK DEPEND(in: &
!\$OMP\& A(JJ:JJ+JJB-1,J:J+JB-1),\&
!\$OMP\& A(K:K+KB-1,J:J+JB-1))
!$OMP& DEPEND(inout: &
!\$OMP\& A(JJ:JJ+JJB-1,K:K+KB-1))
      CALL DGEMM( ... )
!$OMP END TASK
    END DO
  END DO
!$OMP END SINGLE
END DO
!$OMP END PARALLEL
```



#### **Performance numbers**



problem size: n = 10,000, block size: nb = 256

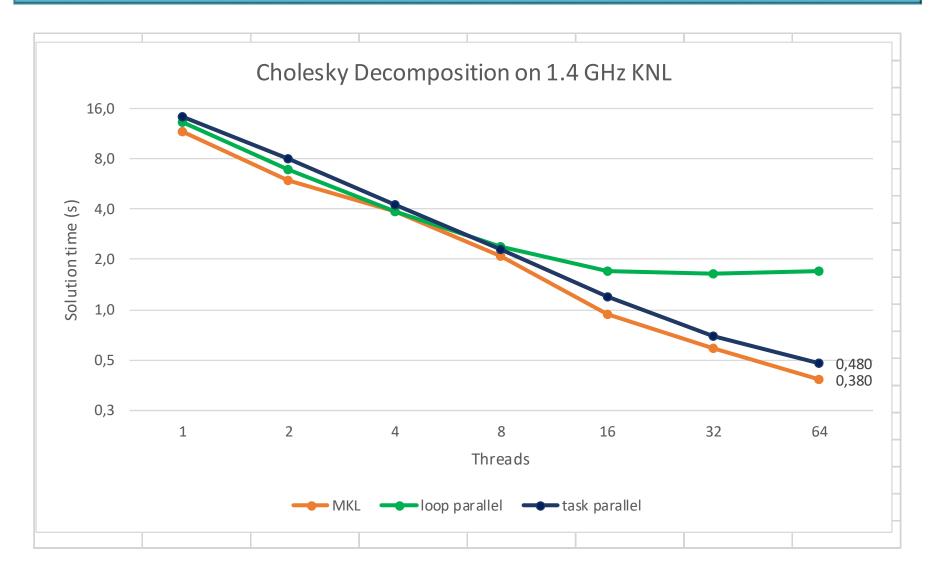




#### **Performance numbers**



problem size: n = 10,000, block size: nb = 256





# Technology advances ...



# Comparing the N = 6000 solution time

	KSR1 (24 cells)	Haswell (28 cores)	KNL (64 cores)
year of release	1992	2014	2015
solution time (s)	270	0.13	0.16
GFlop/s	0.267	566	440
	memory limit of machine		strong scaling limit



# Applying tasking to loops <





#### Tasking and worksharing loops:

- coexistence is difficult, because tasks are often issued in a context that does not permit application of "omp do/for"
- creating a task for each loop iteration may be too fine-grained
- New construct: taskloop

```
!$omp taskloop [clauses]
do var = ni, ne
...
end do
!$omp end taskloop

#pragma omp taskloop [clauses]
for (var = ni; var <= ne; var++) {
...
}</pre>
C
```

creates task regions for iterations of associated loop(s)



# Taskloop clauses



#### Scoping:

- private, firstprivate, shared, default
- Inherited from work sharing:
  - collapse, lastprivate
- Inherited from tasking:
  - if, final, mergeable, priority, untied
- New clauses:
  - grainsize(size)
  - num\_tasks(num)
  - nogroup

constrains number of iterations assigned to each task (upper limit < 2\*grainsize)

is limited

Current compiler support

maximum number of tasks created

by default, a taskloop construct **implies** a taskgroup region. This is similar to the sync at the end of a worksharing construct. The nogroup clause **removes** this additional synchronization.



#### Reductions across tasks

#### Known reduction properties:

- operation and involved variables
- scope of clause: well defined starting point for creating private copies, and end points (usually with synchronization) for putting together partial results



- the second property is not trivially assured in the context of tasking
- it is not obvious which created tasks participate in a reduction

#### Two step procedure for reductions across tasks:

1. define the scope of the reduction (2 variants; note the synchronization point)

```
      !$omp parallel reduction(task, +:x)
      !$omp taskgroup task_reduction(+:x)

      ... ! create tasks (see below)
      !$omp end parallel

      !$omp taskgroup task_reduction(+:x)
      ... ! create tasks (see below)

      !$omp end taskgroup
      !$omp end taskgroup
```

2. inside the region, specify which explicit tasks participate:

```
!$omp task in_reduction(+:x)
...! tasked code & data
!$omp end task

Now: 6th exercise session
```





# **Performance:**

# **Architectural aspects**



#### We need ideas on ...



#### What can be expected from the processor architecture?

- want at least an estimate for performance limits → avoid "stumbling in the dark"
- much more detailed node performance engineering and modeling: course by G. Hager and G. Wellein – see

http://moodle.rrze.uni-erlangen.de/moodle/course/view.php?id=300&username=guest&password=guest&lang=en
and references cited within

#### How to exploit the architecture as best as possible

- use optimal data access patterns
- minimize synchronization overhead
- Account for interactions of OpenMP features with "serial" optimization techniques (might be compiler optimization or lack thereof!)

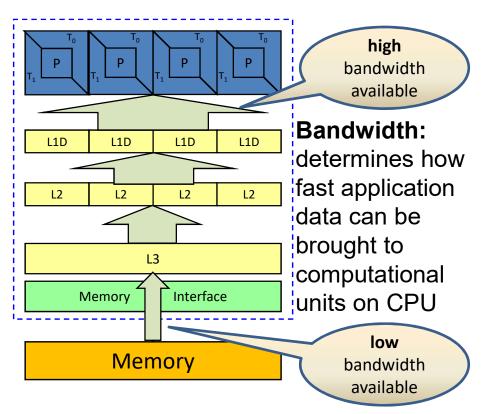


#### **Processor Architecture**



#### Performance Characteristics

 determined by memory hierarchy



- Impact on Application performance: depends on where data are located
  - temporal locality: reuse of data stored in cache allows higher performance
  - no temporal locality: reloading data from memory (or high level cache) reduces performance
- For multi-core CPUs,
  - available bandwidth may need to be shared between multiple cores
    - → shared caches and memory



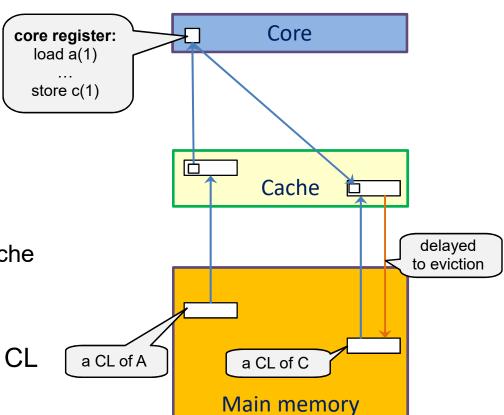
#### **Concept of cache**



- A small but fast memory area
  - used for storing a (small)
     memory working set for efficient
     access

Reasons:

- physical and economic limitations
- Loads (stores) to (from) core registers
  - may trigger cache miss >
    transfer of memory block ("cache line", CL) from memory
- Cache fills up ...
  - usually least recently used CL is evicted



**Example:** c(:) = a(:) + ...





# Control of Affinity NUMA effects False Sharing

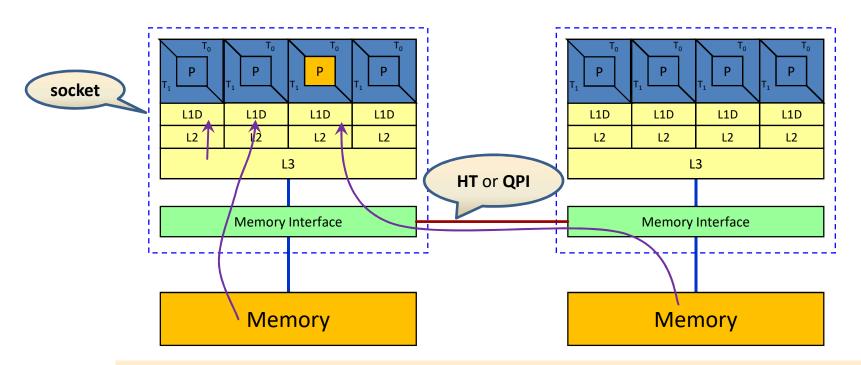


#### **Current Node architecture ...**



- multi-core multi-threaded processors with a deep cache hierarchy
- typically, two sockets per node

Illustration shows 4 cores per socket. Current sockets have 8 – 14 cores



ccNUMA architecture: "cache-coherent non-uniform memory access"



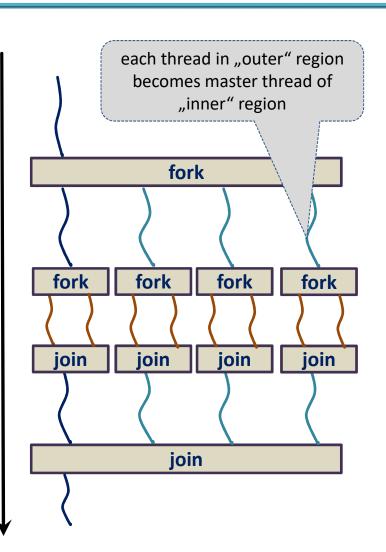
#### Prolegomenon: nested parallelism



An implementation might support this:

nesting of parallel regions

mentioned here for illustrative purposes



execution sequence



#### **Resource assignment**



#### Suitable environment settings

```
one integer for each nesting level

export OMP_NUM_THREADS=4,2
export OMP_NESTED=true else, "inner" regions might/will execute with 1 thread only.

./my_nested_openmp_program.exe forbid implementation to interfere with number of threads assigned
```

#### Operating system:

- responsible for assigning hardware resources to threads
- in general not trivial note that (active) thread count can change during execution

#### Possible issues (performance impact):

- threads might move around between cores
- multiple threads might share a core (or other resources)

→ a mechanism for controlling thread affinity / binding is desirable



#### Thread affinity – Processor binding



#### Two aspects:

- 1. What entity should a thread be bound to? → concept of place
- 2. How should the binding be performed (if at all ...)?
- Optimal binding strategy depends on machine and application
- Putting threads far apart ("spread", "scatter") might
  - improve aggregate memory bandwidth
  - improve combined cache size
  - decrease performance of synchronization constructs
- Putting threads close together (i.e. on two adjacent cores) might
  - improve performance of synchronization constructs
  - decrease available memory bandwidth and cache size per thread
    - → available since **OpenMP 4.0** before that: implementation-specific mechanisms



## OpenMP place: a container unit for pinning of threads

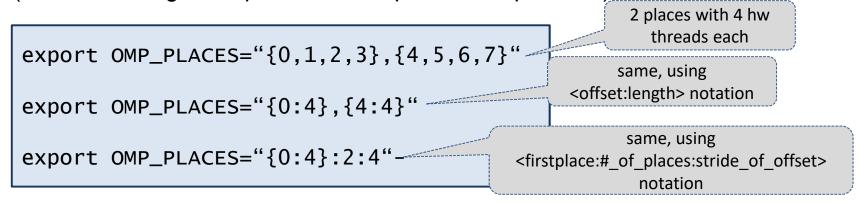


#### Places are defined via either

 an abstract name (threads, cores, or sockets), optionally followed by a bracketed positive integer (number of places):

```
export OMP_PLACES="cores(8)" 8 places with 1 physical core each
```

 or an explicit list of places, specified as list of integer intervals (in the following example, all three specs are equivalent)



meaning of the index is **implementation defined**, but you can expect the smallest unit of execution (a hardware thread on x86) to be used.



#### **OpenMP** binding



#### Determine whether threads should be pinned

- environment variable OMP\_PROC\_BIND
- with values true or false, or
- a comma-separated list of entries:

master	bind created threads to same place as master thread
close	bind created threads to a place close to the one assigned to the master
spread	use a sparse distribution pattern to bind created threads to places

#### Example:

export OMP\_PROC\_BIND=spread,close

binding is determined for at most two levels of parallel nesting



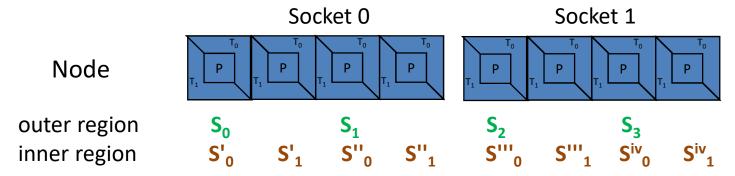
#### **Example for OpenMP binding**



Nested parallelism example from earlier

```
export OMP_NUM_THREADS=4,2
...
export OMP_PLACES="cores(8)"
export OMP_PROC_BIND=spread,close
./my_nested_openmp_program.exe
```

Threads are named S<sub>i</sub>, and S'<sub>i</sub>, S"<sub>i</sub>, ..., for outer and inner region, respectively:



Overcommitment causes places to be reused (i.e. multiple threads per place)



#### Identifying binding strategy within the program



#### The function

<pre>integer() function omp_get_proc_bind()</pre>	Fortran
<pre>omp_proc_bind_t omp_get_proc_bind(void)</pre>	С

#### returns one of the following constants:

omp_proc_bind_false	0
omp_proc_bind_true	1
omp_proc_bind_master	2
<pre>omp_proc_bind_close</pre>	3
omp_proc_bind_spread	4

The value may depend on the nesting level from which the function is called



#### **Identifying placement**



#### A number of functions exist to handle various inquiries:

Name	Result type	Purpose	
<pre>omp_get_num_places()</pre>	int	number of places available	
<pre>omp_get_place_num_procs           (int place_num)</pre>	int	number of processors available in place_num (0 number of places - 1)	
<pre>omp_get_place_proc_ids   (int place_num, int *ids)</pre>	void	ids contains numerical identifiers of processors in place place_num	
<pre>omp_get_place_num()</pre>	int	place number of place to which calling thread is bound	
<pre>omp_get_partition_num_places()</pre>	int	number of places in place partition of innermost implicit task	
<pre>omp_get_partition_place_nums</pre>	void	list of place numbers for innermost implicit task	



#### **Program-internal binding**



- A proc\_bind clause can be specified
- Example:

```
#pragma omp parallel num_threads(4) proc_bind(spread)
    #pragma omp parallel num_threads(2) proc_bind(close)
   executed with
                            Socket 0
                                                    Socket 1
OMP_PLACES=cores(8)
       Node
    outer region
    inner region
```



#### Identifying node topology



#### Topology =

- Where in the machine does core #n reside?
- awkward numbering anyway?
- which cores share which cache levels
- which hardware threads ("logical cores") share a physical core?

#### Use LIKWID tool to identify

- developed by J. Treibig
- https://github.com/RRZE-HPC/likwid has source code and documentation

#### Available commands

- likwid-topology: Print thread and cache topology
- likwid-pin: Pin threaded application without touching code

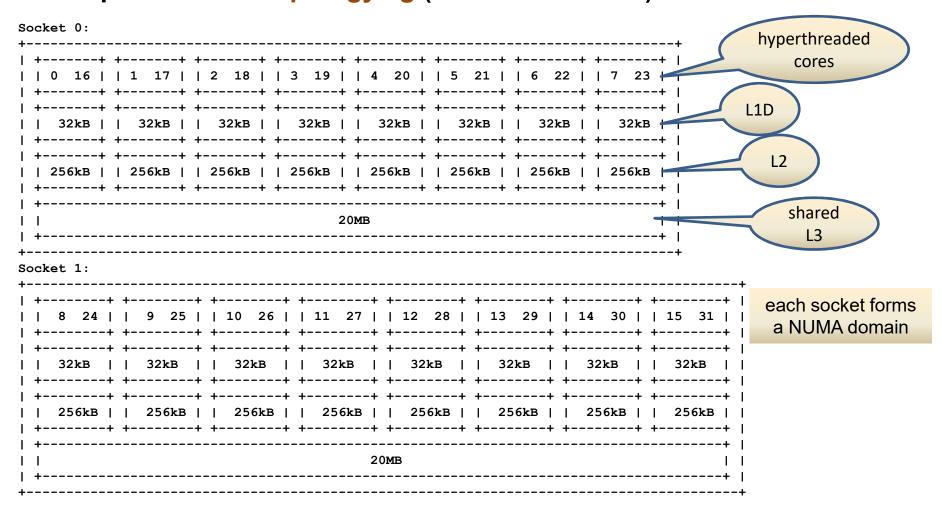
- likwid-perfctr: Measure performance counters
- likwid-mpirun: mpirun wrapper script for easy LIKWID integration
- likwid-bench: Low-level bandwidth benchmark generator tool
- ... some more



#### Intel / Sandy Bridge topology



#### Output of likwid-topology –g (ASCII art section):

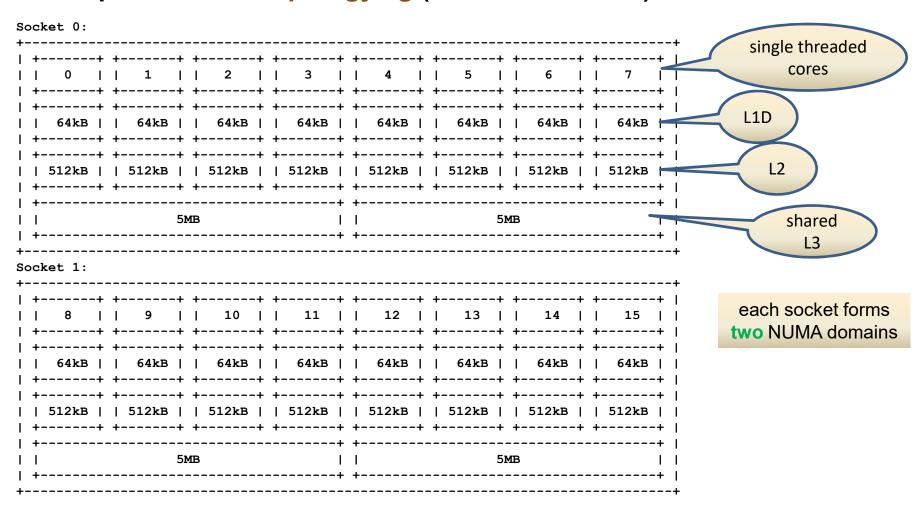




#### **AMD / Magny Cours topology**



#### Output of likwid-topology –g (ASCII art section):





#### likwid-pin – Overview



- Pins processes/threads to specific cores without touching code
  - Directly supports pthreads, gcc OpenMP, Intel OpenMP
  - Based on combination of wrapper tool together with overloaded pthread library >> binary must be dynamically linked!
- Can also be used as a superior replacement for Linux command taskset
- Supports logical core numbering within a node and within an existing CPU set
  - Useful for running inside CPU sets defined by someone else, e.g., the MPI start mechanism or a batch system
- Usage examples:
  - Physical numbering (as given by likwid-topology):

```
likwid-pin -c 0,2,4-6 ./myApp parameters
```

Logical numbering by topological entities:

likwid-pin -c S0:0-3 ./myApp parameters



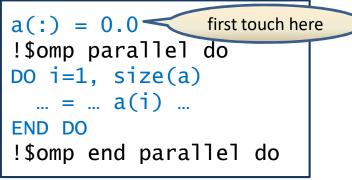
#### **Memory affinity**



all of a(:) physically located here

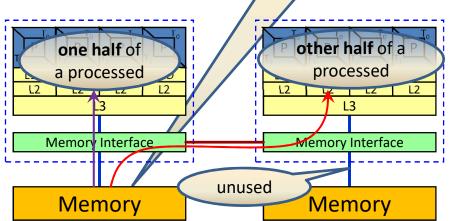
- Allocation of memory (with C malloc() / Fortran ALLOCATE)
  - only provides a virtual memory address
- Physical memory
  - is assigned when a memory location is initialized ("first touch")
  - units of pages (note overhead due to page faults!)
- Consequence for OpenMP
  - possible memory accesses across socket boundaries

Fortran



only half the available

memory BW might be exploited on a 2-socket system



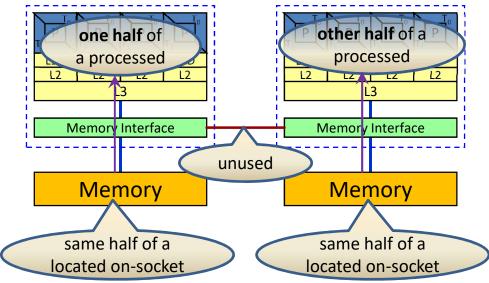


#### **Balancing memory affinity**



- Desirable and scalable memory access pattern:
  - requires initialization with an OpenMP parallelized loop
- Distributed first touch
  - ideally, uses same loop schedule as later processing

```
!$omp parallel do
DO i=1, size(a)
  a(i) = ...
END DO
!$omp end parallel do
...
!$omp parallel do
DO i=1, size(a)
  ... = ... a(i) ...
END DO
!$omp end parallel do
```



 now, the full available memory BW can be exploited on a multi-socket system

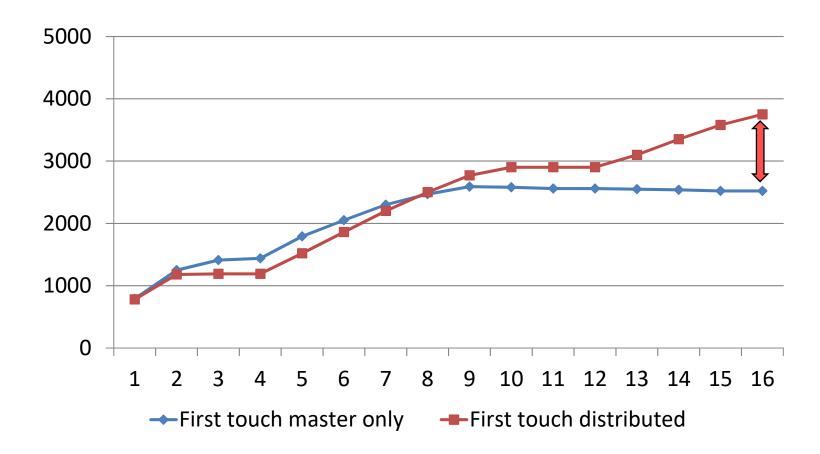


#### **MVM** performance for N=8000



#### Measured on two AMD Magny Cours sockets

thread pinning uses "close" strategy





#### **Tasking and NUMA effects**



#### Remember:

 tasking decouples data items and associated functions from the threading model

```
#pragma omp task
  execute_my_function(a, b, c);
```

#### Consequence:

 repeated execution of tasking on data items might use different threads → memory affinity will get lost!

```
#pragma omp task shared(a, b, c)
    establish_my_data(a, b, c);
#pragma omp taskwait
#pragma omp task shared(a, b, c)
    execute_my_function(a, b, c);
this function might execute on a different thread than this one
```

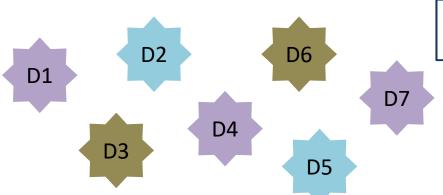


#### Partial therapy: register locality



#### At initialization

store which thread performed it – threads are color coded below



thread	0	1	2
item#	1	2	3
item#	4	5	6
item#	7	-	-

#### Working on data items

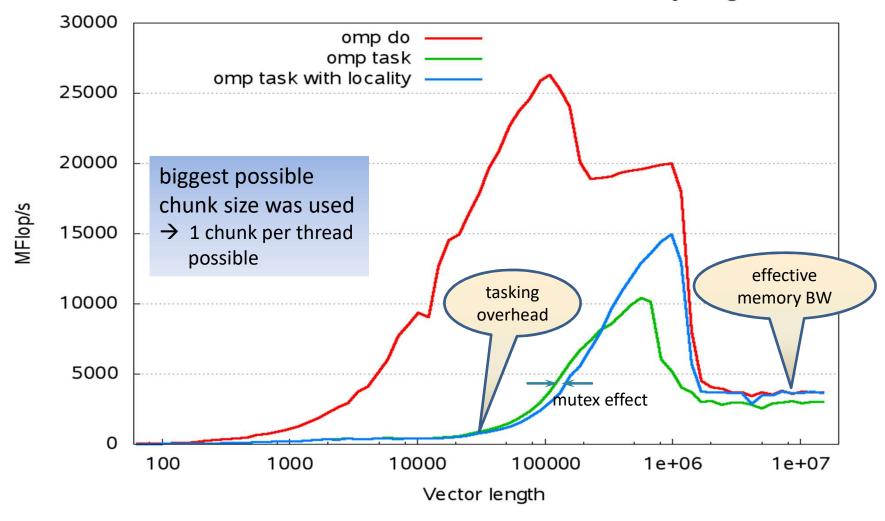
- first work on items that are local to the executing thread
- next work on items that are located elsewhere (nearby first)
  - > task stealing due to unpredictable thread assignment
- additional bookkeeping (mutual exclusion) is needed to assure complete and unique execution



#### Simple example: NUMA-aware tasked triads



#### work shared vector triad with 16 threads on Sandy Bridge





## Performance problems with small shared variables



Example program: count even and odd array values

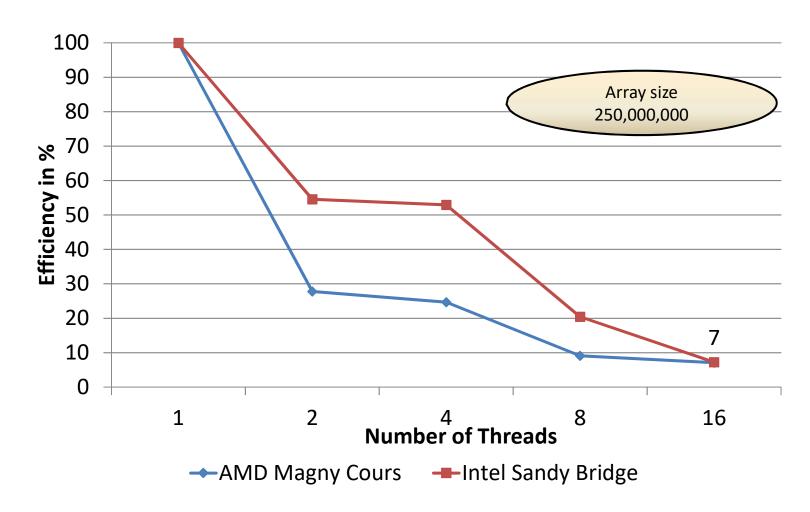
```
integer is(2), ict(2,ntdm), ia(n)
                                      initialization omitted
!$omp parallel private(myid) shared(ict, ia)
  myid = omp_get_thread_num()+1
!$omp do private(index)
  do i=1,n
    index = mod(ia(i), 2)+1
    ict(index,myid) = ict(index,myid) + 1
  end do
                                    formally correct,
!$omp end do
                                    no race condition
!$omp critical
  is = is + ict(1:2, myid)
!$omp end critical
!$omp end parallel
                                                 Fortran
```



#### **Example program parallel efficiency**



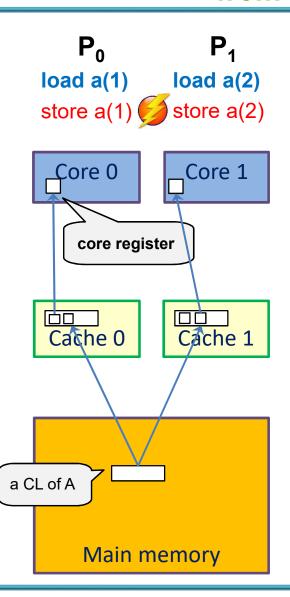
Baseline 1 thread execution time: AMD 0.75 s, Intel SandyBridge 0.37 s





## Updating neighbouring data from different cores





#### Store operation

- write back always done on complete cache lines
- "merging of partial cache lines" is not possible

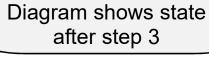
#### Cache coherence protocol

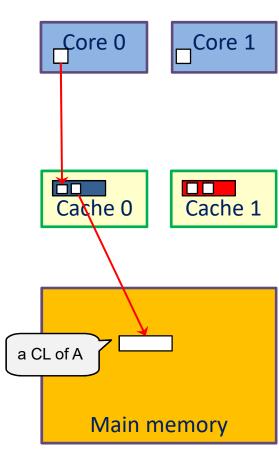
- keeps track of cache line status
- assures data consistency by enforcing hardware synchronization between writes



#### Typical sequence of write operations







### Hardware execution sequence for write on Core 0:

- Request exclusive access to CL (Core 0 issues it first)
- Invalidate CL in Cache 1
- Modify CL in Cache 0 (exclusively owned)
- 4. mark CL shared

#### Hardware execution sequence on Core 1:

- 5. Request CL from memory for reading (granted after CL is marked shared)
- Request exclusive access to CL
- 7. Invalidate CL in Cache 0
- 8. Modify CL in Cache 1 (exclusively owned)
- 9. mark CL shared



#### Consequences



- Repeated access to data in same cache line:
  - causes thrashing of cache lines
  - for each access, more than twice the memory latency may be accumulated, resulting in significant performance reduction
- This effect is called "false sharing"



#### **Avoidance of false sharing**



Privatization – here through use of a reduction variable

```
integer is(2), ia(n)
                                         initialization omitted
!$omp parallel shared(ict, ia)
!$omp do private(index) reduction(+:is)
  do i=1,n
                                      private variables are assured
    index = mod(ia(i), 2)+1
                                      of using well-separated
     is(index) = is(index) + 1
                                      parts of the physical memory
                                      (thread-individual stack or
  end do
                                      heap)
!$omp end do
!$omp end parallel
                                                     Fortran
```

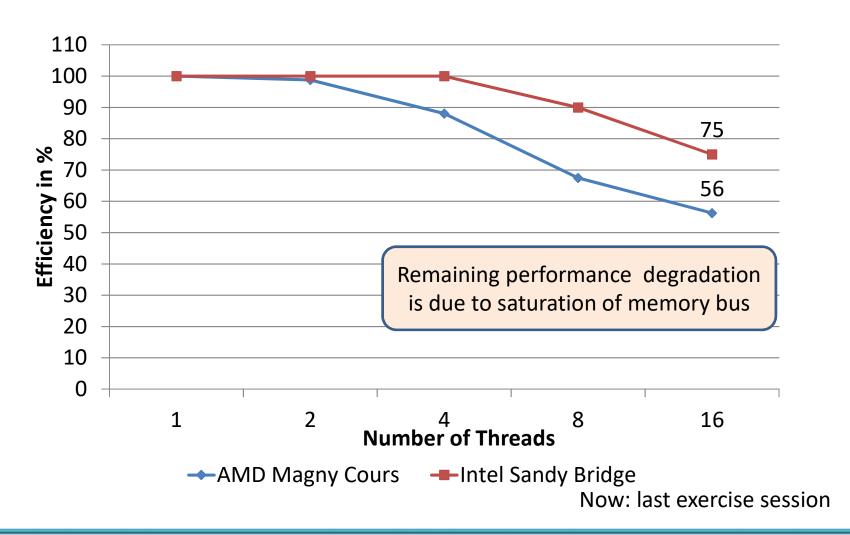
- Alternative for retaining shared variables: Add padding
  - tradeoff: may lose spatial locality



#### Parallel efficiency for improved example



Baseline 1 thread execution time: AMD 0.81 s, Intel SandyBridge 0.36 s







## Outlook: Towards quantifying performance



## Using synthetic loop kernels for performance evaluation



#### Characteristics

- known operation count, load/store count
- some variants of interest:

Kernel	Name	Flops	Loads	Stores
$s = s + a_i * b_i$	Scalar Product	2	2	0
$n^2 = n^2 + a_i * a_i$	Norm	2	1	0
$a_i = b_i * s + c_i$	Linked Triad (Stream)	2	2	1
$a_i = b_i * c_i + d_i$	Vector Triad	2	3	1

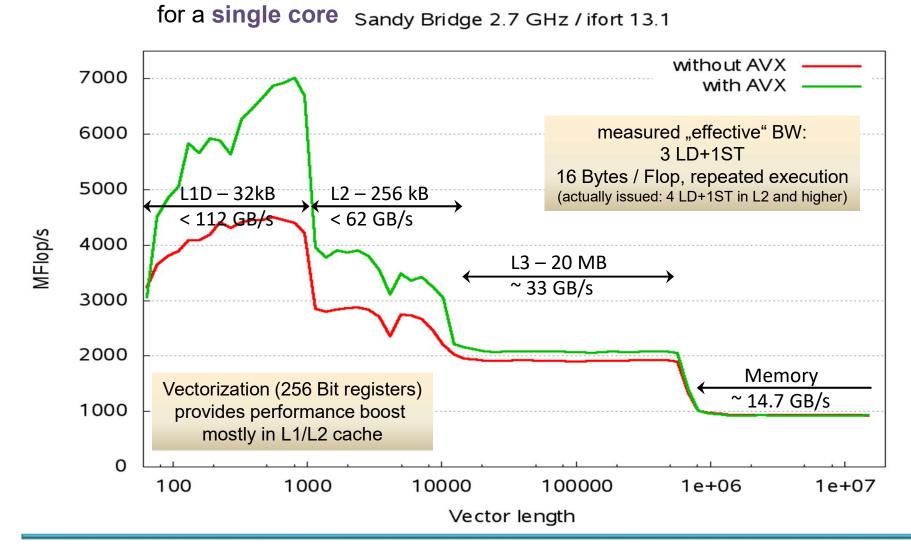
run repeated iterations for varying vector lengths (working set sizes)



#### **Vector Triad D(:) = A(:) + B(:) \* C(:)**



Synthetic benchmark: bandwidths of "raw" architecture



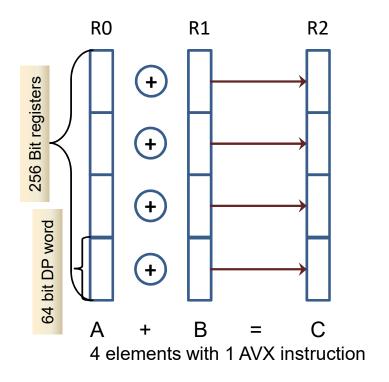


#### **Theoretical performance limit**



#### Sandy Bridge vector unit:

- 256 Bit SIMD (single instruction multiple data)
- Example: addition of 8 Byte words



#### Instruction capability

 1 vector add and 1 vector mult per cycle → theoretical Peak 8 Flops/cycle

#### LD/ST issue capability

- 4 Words LD/cycle
- 4 Words ST/(2 cycles)

Only L1 might maintain needed bandwidth

#### Vector triad:

 required loads limit performance to 8 Flops / 3 cycles

i.e. **7.2 GFlop/s** at 2.7 GHz

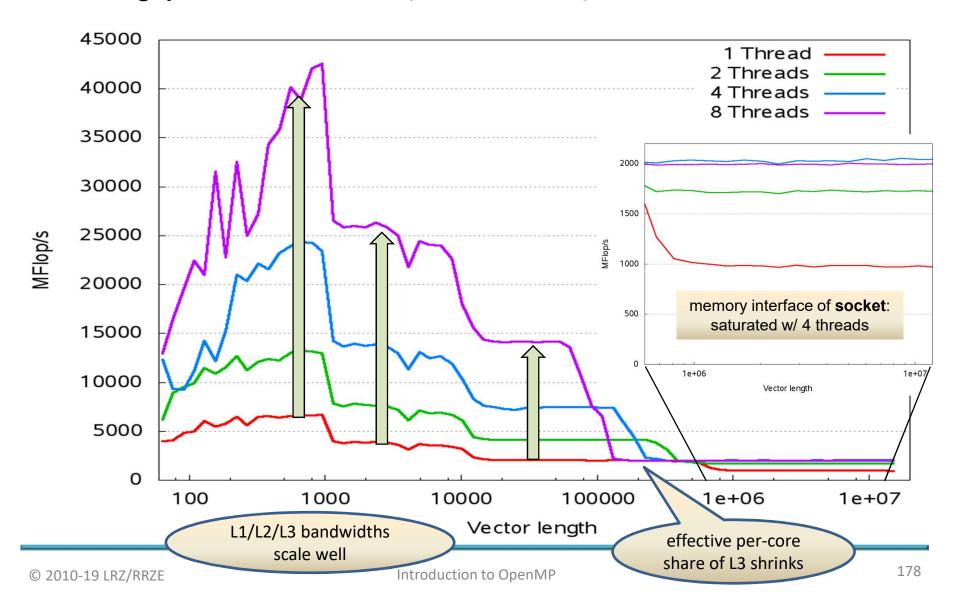
 Consult processor-specific architecture manual



#### **Vector Triad D(:) = A(:) + B(:) \* C(:)**



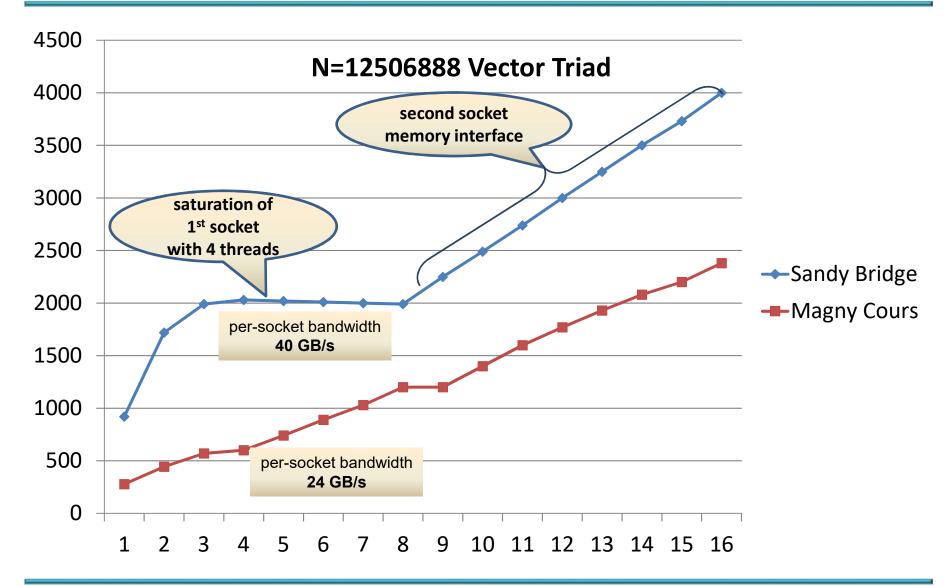
■ Throughput mode: run with independent threads up to number of cores on a socket





#### **Looking at Memory Performance**





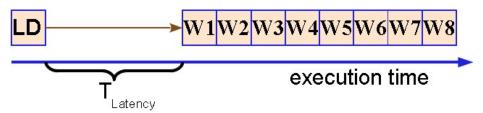


#### More on cache-based memory systems



#### Loads and Stores

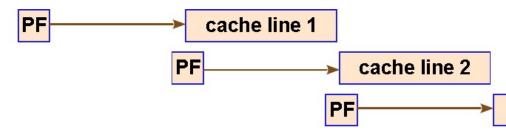
usually apply to cache lines



size: 64, 128 or more Bytes

#### Pre-fetch

 avoid latencies when streaming data



execution time

- pre-fetches usually done in hardware
- decision according to memory access pattern

#### **Pre-Requisite:**

cache line 3

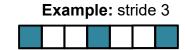
- spatial locality
- violation of spatial locality:
   if only part of a cache line is used
   → effective reduction in
   bandwidth

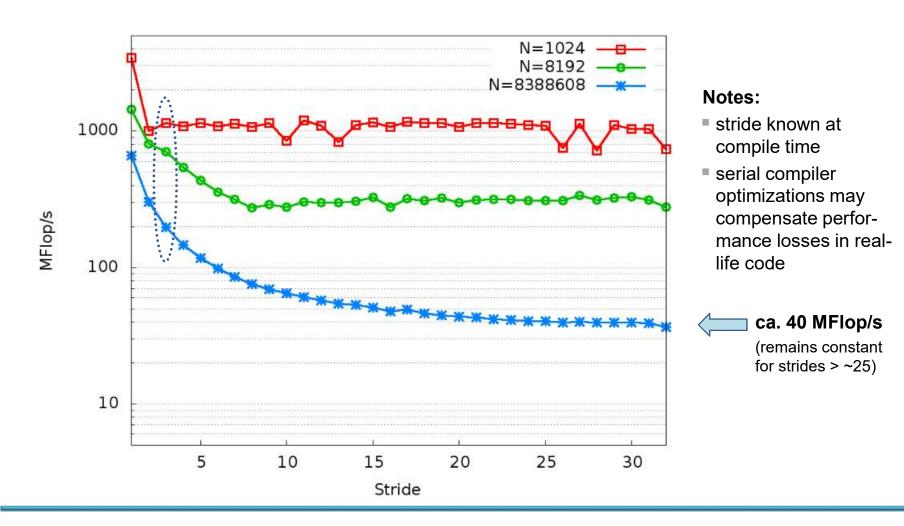


# Performance of strided triad on Sandy Bridge - loss of spatial locality



D(::stride) = A(::stride) + B(::stride) \*C(::stride)







# Returning to the matrix-vector product



$$\mathbf{r} = \mathbf{M} \cdot \mathbf{x} \text{ i.e. } r_i = \sum_{j=1}^n M_{ij} x_j$$

#### First parallelization attempt:

#### Parallel patterns used:

- data decomposition (load balanced)
- loop parallelism (no dependencies)

#### Directive placement:

 coarse grained parallelism to avoid synchronization overhead

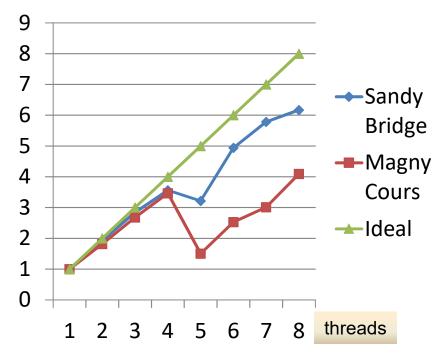


# Measured performance (size 8000)



Speed-Up:  $S(n_t) = \frac{T(1)}{T(n_t)}$ 

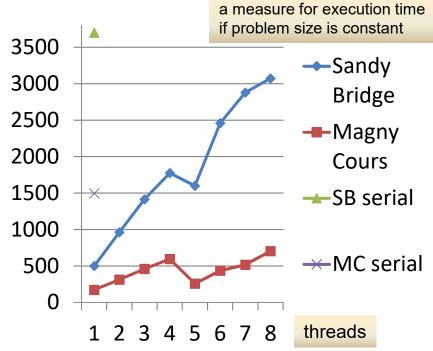
as a function of number of threads on 8-core processors



Scaling bad beyond 4 threads

## Absolute performance:

• MFlop/s =  $2 \cdot n^2$  / time



- used dgemv for serial run
- Speed-Up useless if baseline performance is bad

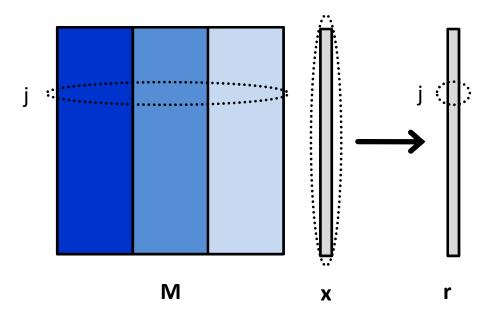


# **Improved Matrix-Vector Multiply**



#### Switch loop order

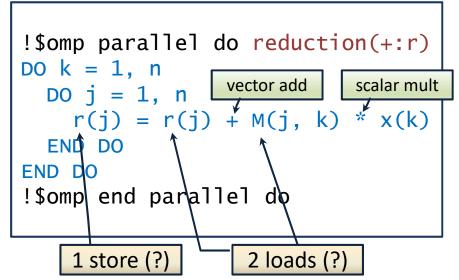
map column blocks to threads:



 color code indicates thread assignment

#### Variant 2 of code:

- contiguous access to M
- array reduction on result vector



# Performance estimate for single thread:

double that of triad → 1.86 GFlop/s

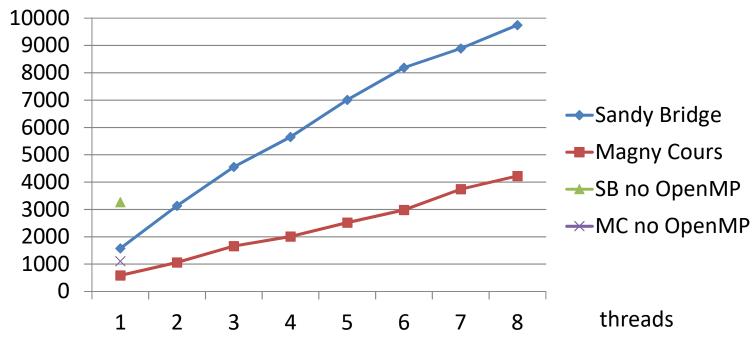
Cannot be the whole truth – remember serial performance: 3.7 GFlop/s!



# Re-measured performance (size 8000)



For variant 2 of the MVM: Performance in MFlop/s



#### Comments:

- "no OpenMP" → variant 2 compiled without OpenMP
- Conclusion: compiler stops making certain serial optimizations if OpenMP switch is toggled



# Variant 3: Reduce memory traffic



#### Outer loop unrolling

- conditioning omitted
- asymptotically increases intensity to 2 Flops per word (1 load on matrix per original loop iteration)

Unrolling is **limited** by number of available registers and prefetch streams (architecture-dependent!)

#### Expected performance

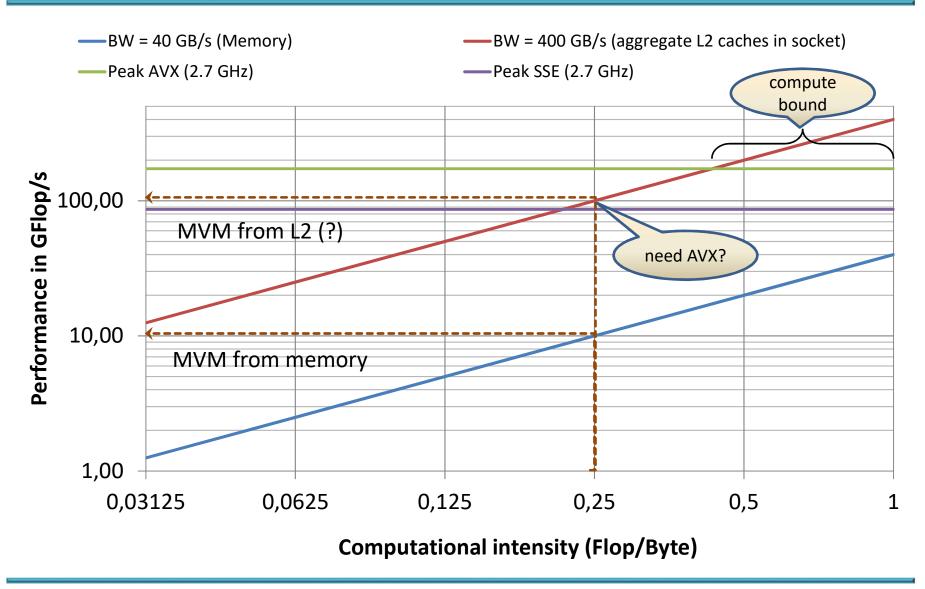
- for M from memory (i.e. outside any cache)
- contiguous streaming of data
- assuming 40 GB/s bandwidth for a socket

 estimation method is known as "Roofline Model"



# **Graphical representation of Roofline**



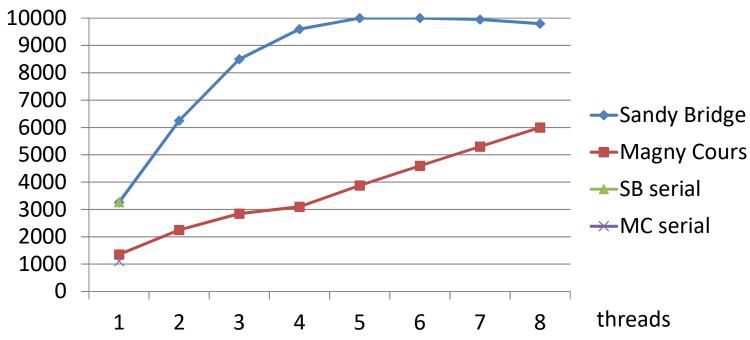




# **Variant 3 MVM performance (N=8000)**



In MFlop/s. Unroll factors: Sandy Bridge 4, Magny Cours 8



#### Comment:

- roofline model only predicts "saturated" performance
- single-thread performance is limited by non-overlapping memory/core operations (see ref. (2))



# Why use variant 3 ...



- ... if variant 2 gives us the full performance anyway?
  - even if this only is attained with 8 threads

#### Possible reasons:

- "switch off" cores 6-8 to save energy (relevant for you if this is budgeted – may happen not too far in the future!)
- use cores 6-8 for other tasks that are cache bound
- use cores 6-8 for MPI communication (I/O via PCI) if you do hybrid programming (i.e., combine MPI with OpenMP)





# References



# Recommended reading



- (1) OpenMP 5.0 standard and OpenMP 4.5 examples at <a href="http://www.openmp.org/specifications/">http://www.openmp.org/specifications/</a>
- (2) Parallel programming in OpenMP
  Rohit Chandra et al; Morgan Kaufmann 2000
- (3) Using OpenMP portable shared memory parallel programming B. Chapman, G. Jost, R. van der Pas; MIT Press 2008
- (4) Using OpenMP the next step
  R. van der Pas, E. Stotzer. Ch. Terboven; MIT Press 2017
- (5) J. Treibig, G. Hager, G. Wellein: LIKWID

  A lightweight performance-oriented tool suite for x86 multicore environments.

  PSTI2010, Sep 13-16, 2010, San Diego, CA DOI: 0.1109/ICPPW.2010.38; Preprint: <a href="http://arxiv.org/abs/1004.4431">http://arxiv.org/abs/1004.4431</a>
- (6) G. Hager, J. Treibig, J. Habich, and G. Wellein:
  Exploring performance and power properties of modern multicore chips via simple machine models. Preprint: arXiv:1208.2908
- (7) G. Hager, G. Wellein: Introduction to High Performance Computing for Scientists and Engineers. Chapman & Hall / CRC (2011)





# Appendix: Setting up Vtune Amplifier



## **Using Vtune Amplifier on x86-based systems**



#### Tuning of serial and threaded programs

performance counter access requires group rights

#### Start up GUI

- prerequisites: set up environment and possibly stack limit
- then, invoke the GUI with amplxe-gui &
- command line amplxe-cl is also available, but will not be discussed
- Project generation analogous to Intel Inspector



# **Example run: A badly performing** solution of the histogram calculation

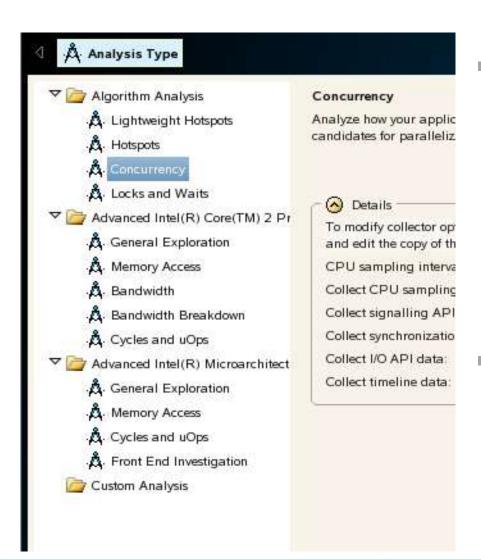


```
#pragma omp parallel private(seed,i,k,me)
    me = omp_get_thread_num();
    seed = 123 + 159*me;
    for (k=0; k<100000; ++k) {
#pragma omp for
      for (i=0; i<10000; ++i) {
        ir[i] = rand_r(&seed) & 0xf;
#pragma omp master
      for (i=0;i<10000; ++i) {
        hist[ir[i]]++;
#pragma omp barrier
// prevents ir from being modified
// before hist update is done
```



# **Choose Analysis type**





### Various types are provided

- select "Concurrency"
- in the project properties, set OMP\_NUM\_THREADS to number of physical cores

#### Note:

performance quality evaluation assumes complete system is used

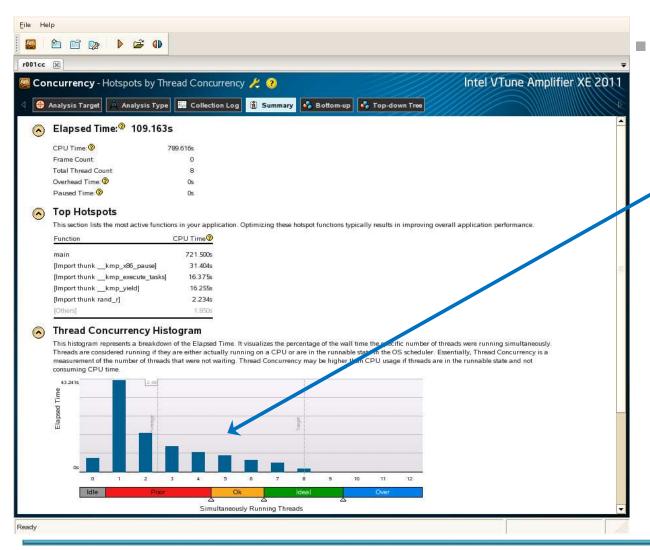
#### Note:

 analysis may take quite a long time to run, even for programs of small size



# **Result tabs: Summary**





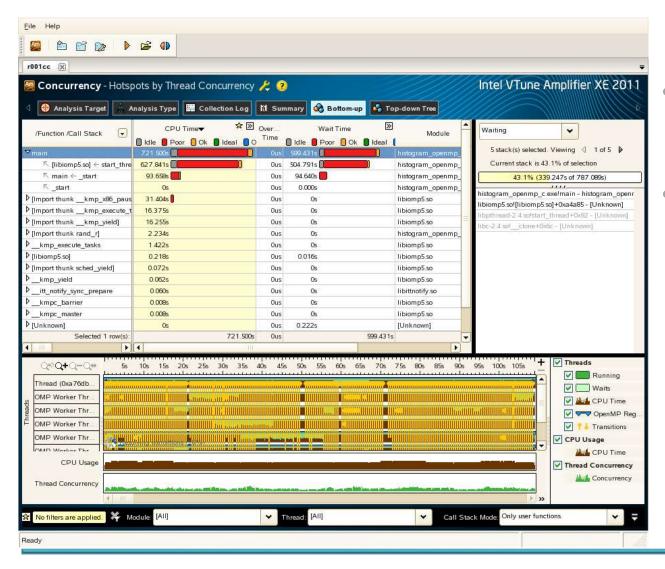
#### Result:

 thread concurrency very low although CPU usage is high



# Result tabs: Bottom-up view





#### **Observation:**

- much time spent in OpenMP run time library
- lots of transitions indicated → have false sharing



#### **Drill down to source**



Click on routine with significant resource usage

