High Performance Computing

Selected topics in shared-memory parallelization

G. Hager, G. Wellein

Regionales Rechenzentrum Erlangen

W. u. E. Heraeus Summerschool

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Another warning

Optimization of sequential code goes first!

Outline

- Architecture of shared memory computers
  - UMA/ccNUMA
  - Cache coherence
- Shared memory programming
  - Introduction to OpenMP
  - Common pitfalls
  - Parallelization of sparse MVM
- Programming for ccNUMA systems
  - Correct page placement
  - Optimization of parallel sparse MVM
  - C++ issues

Architecture of shared memory computers

Shared memory computers: Basic concepts

- **Shared Memory Computer provides single, shared address space for all parallel processors**

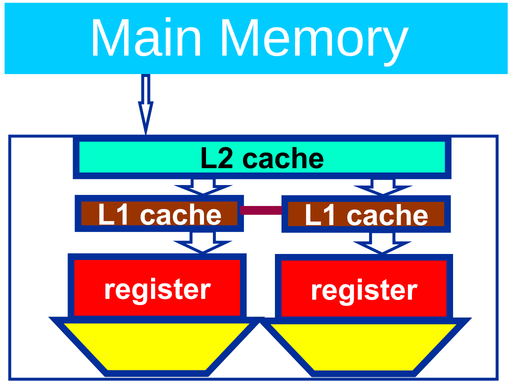
- **Two basic categories of shared memory systems**
  - **Uniform Memory Access (UMA):**
    - **Flat Memory: Memory is equally accessible to all processors with the same performance (Bandwidth & Latency).**
    - **A.k.a Symmetric Multi Processor (SMP) system**

  - **Cache-Coherent Non Uniform Memory Access (ccNUMA):**
    - **Memory is physically distributed: Performance (Bandwidth & Latency) is different for local and remote memory access.**

- **Cache-Coherence protocols and/or hardware provide consistency between data in caches (multiple copies of same data!) and data in memory**

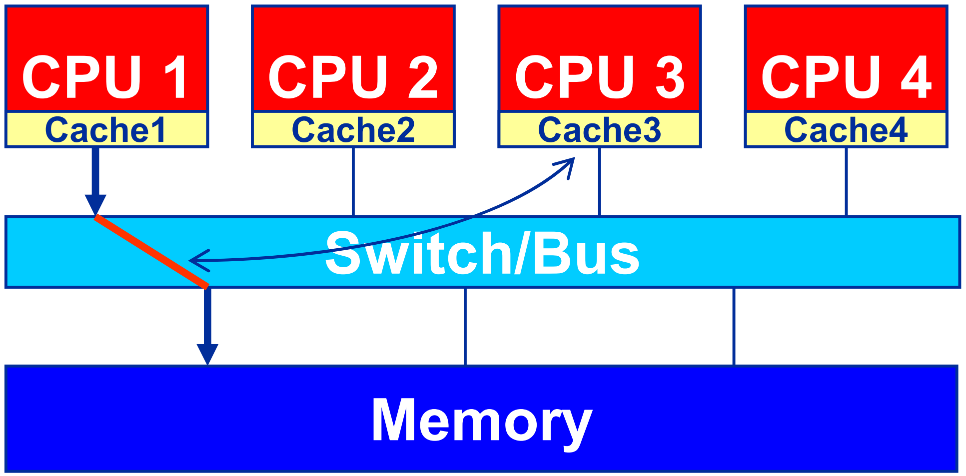
Shared memory computers: UMA

UMA architecture



Simplest implementation: Dual-Core Processor (e.g. AMD Opteron dual-core or Intel Core)

Multi-Processor servers use bus or switch to connect CPUs with main memory

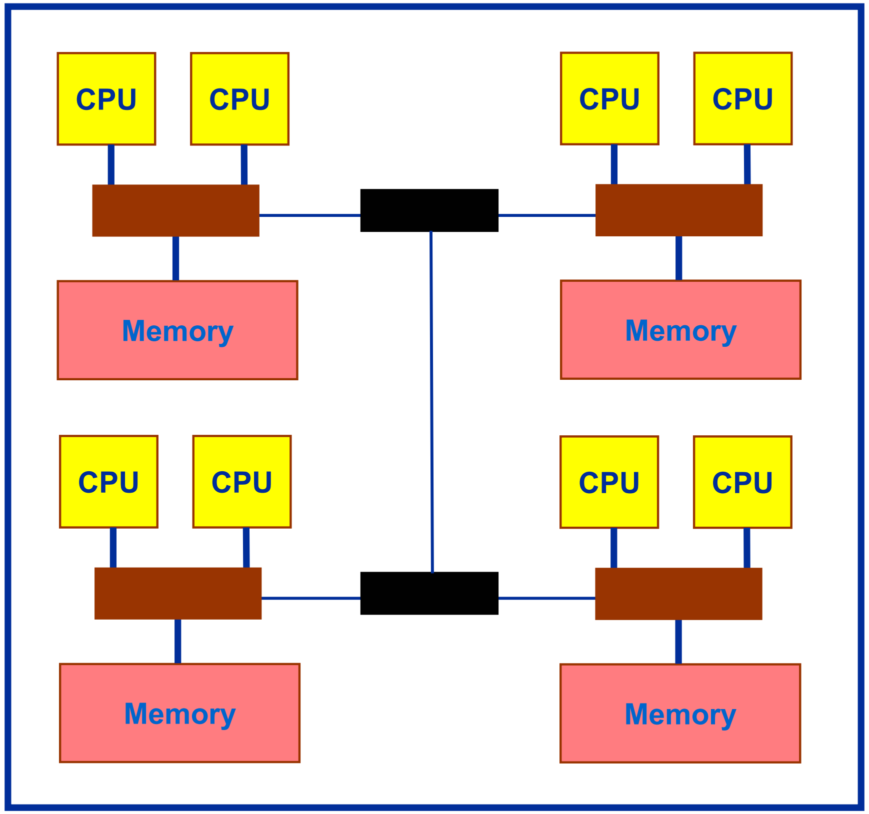


- Bus: Only one processor can access bus at a time!
- Switch: Cache-Coherency traffic can “pollute” switch
- Scalability beyond 2–8 CPUs is a problem
- Dual core chips, small Itanium servers, NEC SX8

ccNUMA architecture

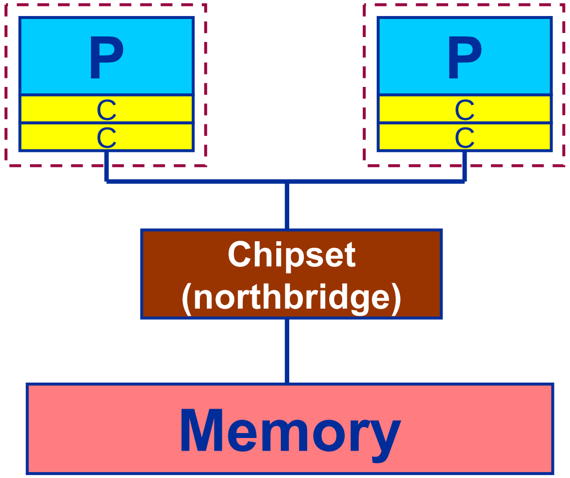
Proprietary hardware concepts (e.g. Hypertransport/Opteron or NUMALink /SGI) provide single address space & cache coherency for physically distributed memory

- Advantages:
  - Scalable concept (systems up to 1024 CPUs are available)
- Disadvantages:
  - Cache Coherence hard to implement / expensive
  - Performance depends on access to local or remote memory
    (no flat view of memory!)

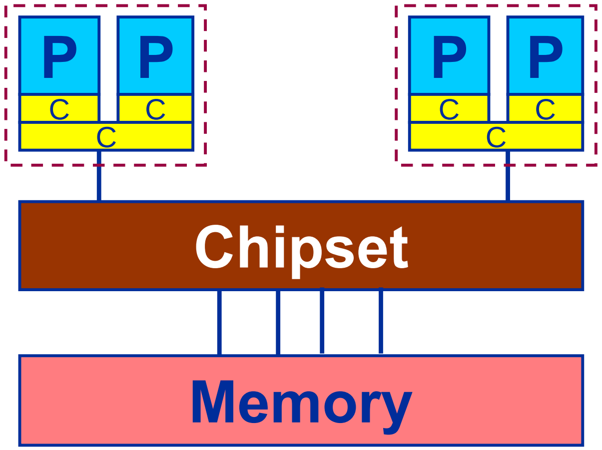


Shared memory computers: Some examples

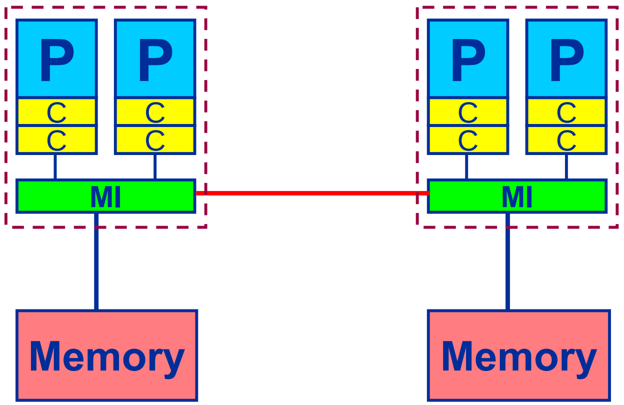
- Dual CPU Intel Xeon node



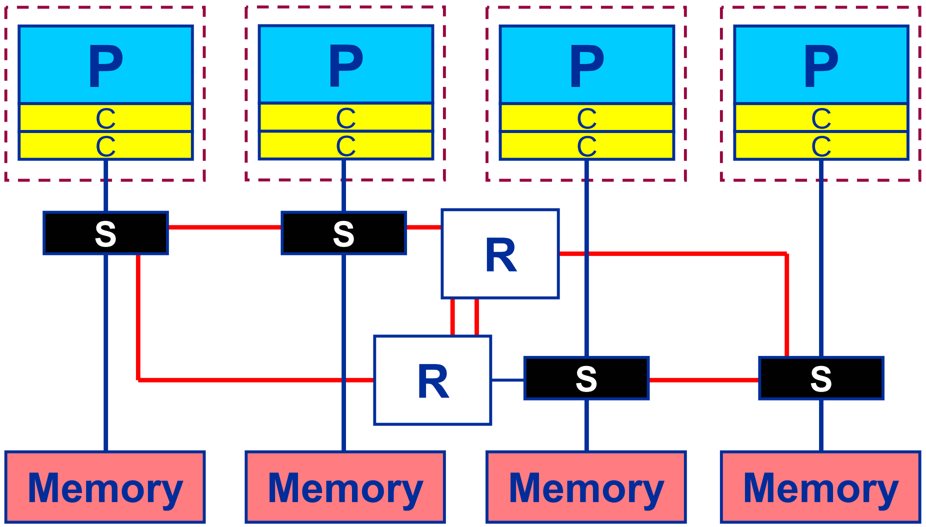
- Dual Intel "Core" node



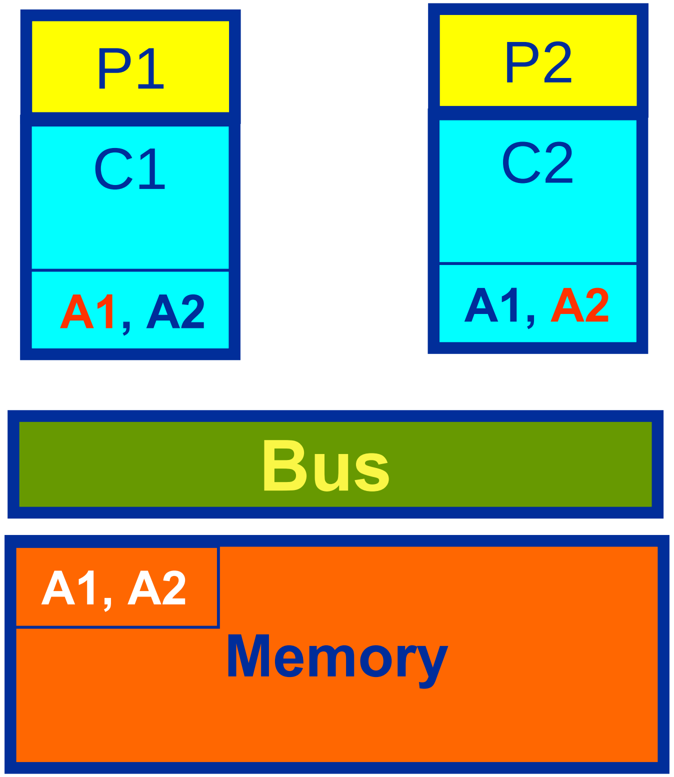
- Dual AMD Opteron node



- SGI Altix (HLRB2 @ LRZ)



- Data in cache is only a copy of data in memory
  - Multiple copies of same data on multiprocessor systems
  - Cache coherence protocol/hardware ensure consistent data view
  - Without cache coherence, shared cache lines can become clobbered:



P1	P2
`Load A1`	`Load A2`
`Write A1=0`	`Write A2=0`

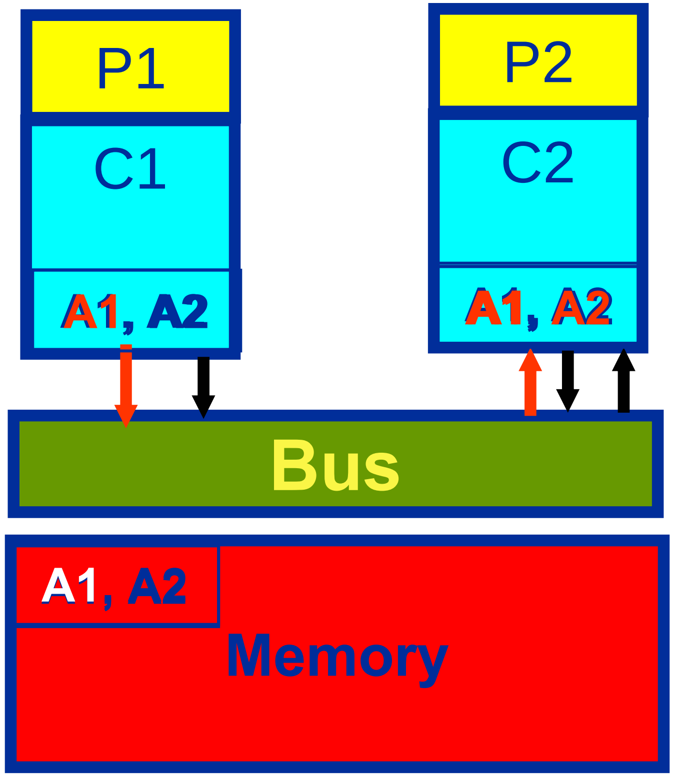
Write-back to memory leads to incoherent data

A1, A2 | A1, A2 | A1, A2

C1 & C2 entry can not be merged to: A1, A2

Shared Memory Computers
Cache coherence

- **Cache coherence protocol must keep track of cache line (CL) status**



P1	P2
`Load A1`	`Load A2`
`Write A1=0:`	
1. Request exclusive access to CL	
2. Invalidate CL in C2	
3. Modify A1 in C1	
	`Write A2=0:`
	1. Request exclusive CL access
	2. CL write back+ Invalidate
	3. Load CL to C2
	4. Modify A2 in C2

t

C2 is exclusive owner of CL ←

- Cache coherence can cause substantial overhead
  - may reduce available bandwidth
- Different implementations
  - Snoopy: On modifying a CL, a CPU must broadcast its address to the whole system
  - Directory, "snoop filter": Chipset ("network") keeps track of which CLs are where and filters coherence traffic
- Directory-based ccNUMA can reduce pain of additional coherence traffic
- But always take care:

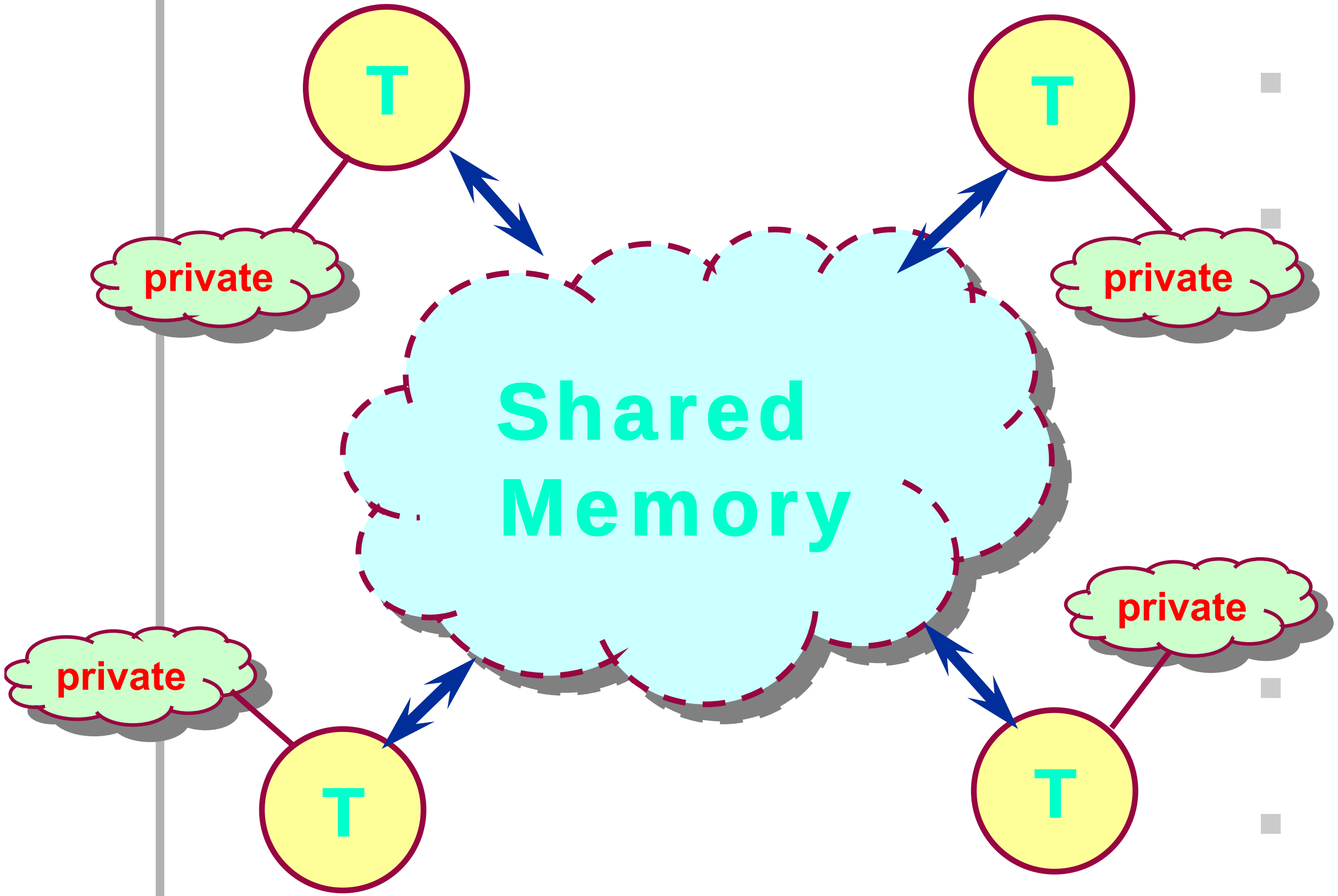
Multiple processors should never write frequently to the same cache line ("*false sharing*")!

Shared-Memory Parallelization

Parallel Programming with OpenMP

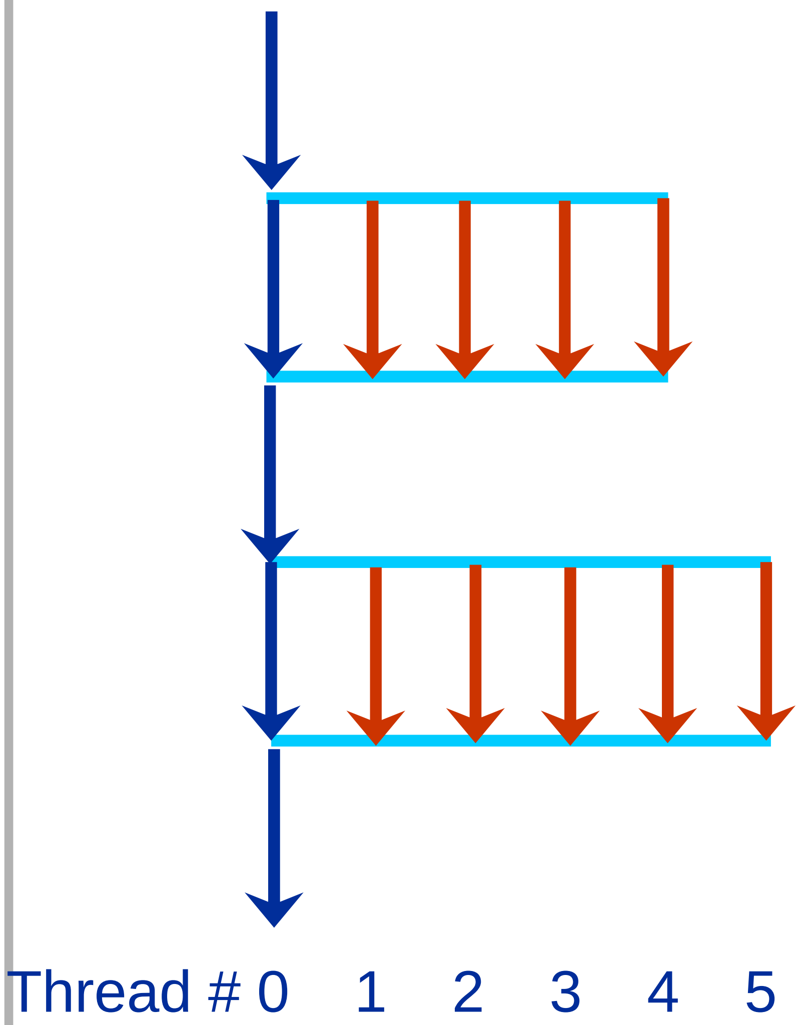
- "Easy" and portable parallel programming of shared memory computers: OpenMP
  - Standardized set of compiler directives & library functions: `http://www.openmp.org/`
    - FORTRAN, C and C++ interfaces are defined
    - Supported by most/all commercial compilers, GNU starting with 4.2
    - Few free tools are available
  - OpenMP program can be compiled and executed on a single-processor machine just by ignoring the directives
    - API calls must be masked out though
  - Supports data parallelism
- Central concept of OpenMP programming: Threads

Shared Memory Model used by OpenMP



- Threads access globally shared memory
- Data can be shared or private
  - shared data available to all threads (in principle)
  - private data only to thread that owns it
- Data transfer transparent to programmer
- Synchronization takes place, is mostly implicit

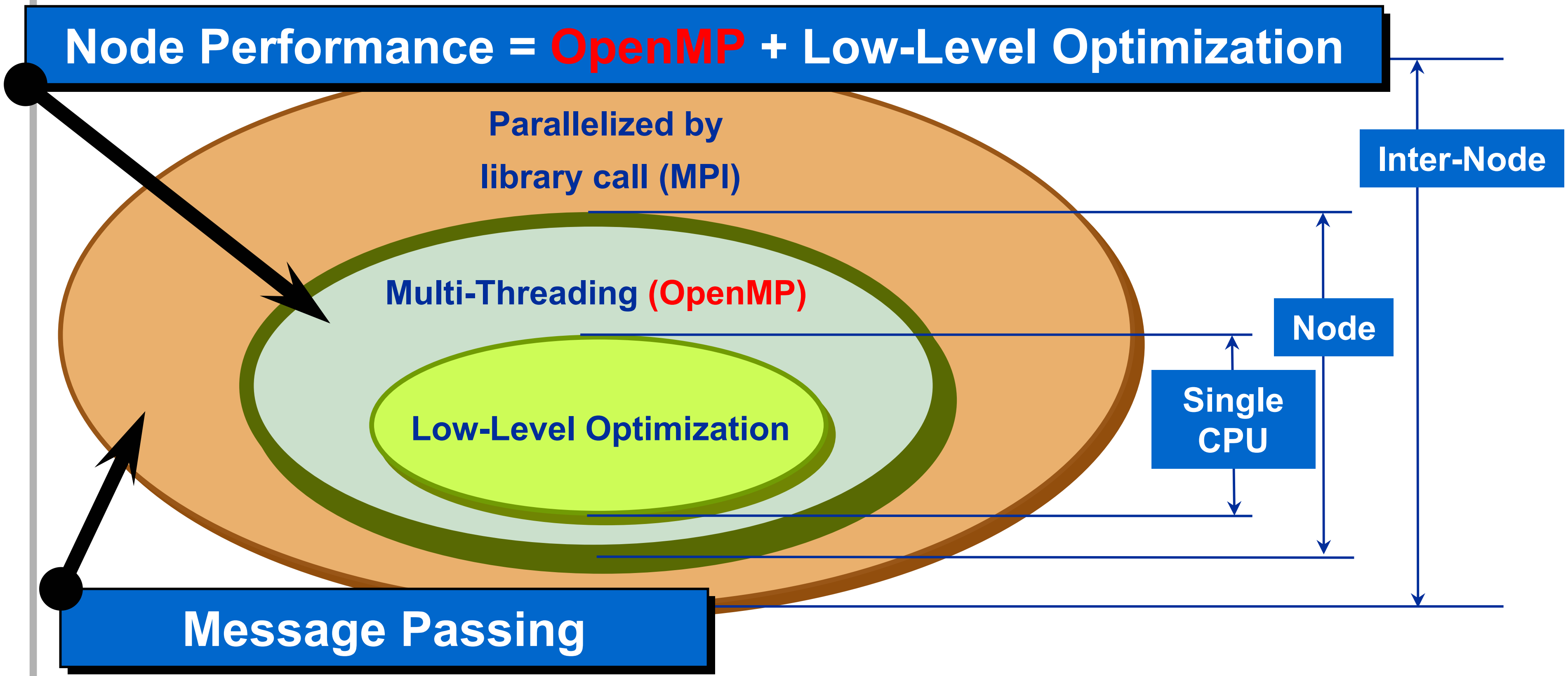
OpenMP Program Execution
Fork and Join



- Program start: only master thread runs
- Parallel region: team of worker threads is generated ("fork")
- synchronize when leaving parallel region ("join")
- Only master executes sequential part
  - worker threads persist, but are inactive
- task and data distribution possible via directives
- Usually optimal:

  1 Thread per Processor

Hybrid parallelization on clustered SMPs



DO l=1,l — Inter-node parallelization (MPI)

DO j=1,m — Intra-node OpenMP processing

DO k=1,n — single processor execution

⋮

Basic OpenMP functionality

About Directives and Clauses

About Data

About Parallel Regions
and Work Sharing

First example: Numerical integration

Approximate by a discrete sum

$$\int_0^1 f(t)\,dt \approx \frac{1}{n}\sum_{i=1}^{n} f(x_i)$$

where

$$x_i = \frac{i-0.5}{n} \quad (i=1,\ldots,n)$$

We want

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

→ **solve this in OpenMP**

```
program compute_pi
...   (declarations omitted)

! function to integrate
f(a)=4.0_8/(1.0_8+a*a)

w=1.0_8/n
sum=0.0_8

do i=1,n
   x=w*(i-0.5_8)
   sum=sum+f(x)
enddo
pi=w*sum

...    (printout omitted)
end program compute_pi
```

First example: Numerical integration

```
...
pi=0.0_8
w=1.0_8/n
!$OMP parallel private(x,sum)
sum=0.0_8
!$OMP do
do i=1,n
  x=w*(i-0.5_8)
  sum=sum+f(x)
enddo
!$OMP end do
!$OMP critical
pi=pi+w*sum
!$OMP end critical
!$OMP end parallel
```

concurrent execution by "team of threads" (the `!$OMP parallel` … `!$OMP end parallel` region)

worksharing among threads (the `!$OMP do` … `!$OMP end do` loop)

sequential execution (the `!$OMP critical` … `!$OMP end critical` section)

OpenMP Directives
Syntax in Fortran

- **Each directive starts with sentinel in column 1:**
  - fixed source: `!$OMP` or `C$OMP` or `*$OMP`
  - free source: `!$OMP`

  followed by a directive and, optionally, clauses.
- **For function calls:**
  - conditional compilation of lines starting with `!$` or `C$` or `*$`

  Example:

```
   myid = 0
!$ myid = omp_get_thread_num()
```

  - **use include file for API call prototypes (or Fortran 90 module `omp_lib` if available)**

- **Include file**

```
#include <omp.h>
```

- **pragma preprocessor directive:**

```
#pragma omp [directive [clause ...]]
  structured block
```

- **Conditional compilation: Compiler's OpenMP switch sets preprocessor macro**

```
#ifdef _OPENMP

... do something

#endif
```

OpenMP Syntax: Clauses

- Many (but not all) OpenMP directives support clauses
- Clauses specify additional information with the directive
- Integration example:
  - `private(x,sum)` appears as clause to the `parallel` directive
- The specific clause(s) that can be used depend on the directive
- Another example: `schedule(…)` clause
  - `static[,chunksize]`: round-robin distribution of chunks across threads (no chunksize: max. chunk size – default!)
  - `dynamic[,chunksize]`: threads get assigned work chunks dynamically; used for load balancing
  - `guided[,chunksize]`: like dynamic, but with decreasing chunk size (minimal size = chunksize); used for load balancing when dynamic induces too much overhead
  - `runtime`: determine by OMP_SCHEDULE shell variable

OpenMP parallel regions
How to generate a team of threads

- `!$OMP PARALLEL` and `!$OMP END PARALLEL`
  - Encloses a parallel region: All code executed between start and end of this region is executed by all threads.
  - This includes subroutine calls within the region (unless explicitly sequentialized)
  - Both directives must appear in the same routine.

- C/C++:

```
#pragma omp parallel
structured block
```

No `END PARALLEL` directive since block structure defines boundaries of parallel region

OpenMP work sharing for loops

Requires thread distribution directive

`!$OMP DO / !$OMP END DO` encloses a loop which is to be divided up if within a parallel region ("sliced").

- all threads synchronize at the end of the loop body
- this default behaviour can be changed ...

- Only loop immediately following the directive is sliced
- C/C++:

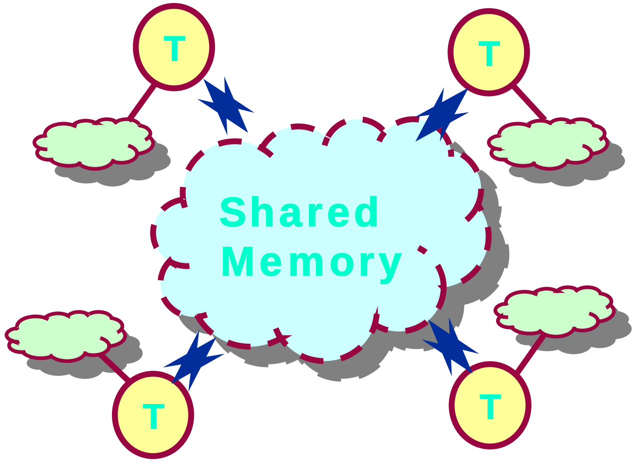
```
#pragma omp for [clause]
for ( ... )  {
         ...
    }
```

- restrictions on parallel loops (especially in C/C++)
  - trip count must be computable (no `do while`)
  - loop body with single entry and single exit point
  - Use integers, not iterators als loop variables

Directives for data scoping: shared and private

- **Remember the OpenMP memory model?**

  Within a parallel region,
  data can either be



- **private to each executing thread**

  → each thread has its own **local copy** of data

  or be

- **shared between threads**

  → there is **only one instance** of data available to all threads

  → this does **not** mean that the instance is always **visible** to **all** threads!

- **Integration example:**
  - **shared scope not desirable for x and sum** since values computed on one thread must not be interfered with by another thread.
  - Hence:

```
!$OMP parallel private(x,sum)
```

Defaults for data scoping

- All data in parallel region is shared
- This includes global data (Module, COMMON)
- Exceptions:
  1. Local data within enclosed subroutine calls are private (Note: Inlining must be treated correctly by compiler!) unless declared with SAVE attribute
  2. Loop variables of parallel (“sliced”) loops are private
- Due to stack size limits it may be necessary to give large arrays the SAVE attribute
  - This presupposes it is safe to do so!
  - If not: make data dynamically allocated
  - For Intel Compilers: `KMP_STACKSIZE` may be set at run time (increase thread-specific stack size)

Changing the scoping defaults

- Default value for data scoping can be changed by using the `default` clause on a parallel region:

```
!$OMP parallel default(private)
```

Not in C/C++

- Beware side effects of data scoping:

  Incorrect `shared` attribute may lead to race conditions and/or performance issues ("false sharing").
  - Use verification tools.
- Scoping of local subroutine data and global data
  - is not (hereby) changed
  - compiler cannot be assumed to have knowledge
- Recommendation: Use

```
!$OMP parallel default(none)
```

  to not overlook anything

Storage association of private data

- Private variables: undefined on entry and upon exit of parallel region

- Original value of variable (before parallel region) is undefined after exit from parallel region
- To change this:
  - Replace `private` by `firstprivate` or `lastprivate`

- Private variable within parallel region has no storage association with same variable outside region

Running an OpenMP program

- **Number of threads: Determined by shell variable**

  OMP_NUM_THREADS

- **Loop scheduling: Determined by shell variable**

  OMP_SCHEDULE

- **Some implementation-specific environment variables exist (here for Intel):**
  - **KMP_STACKSIZE: configure thread-local stack size**
  - **KMP_LIBRARY: specify the strategy for releasing threads that have nothing to do**

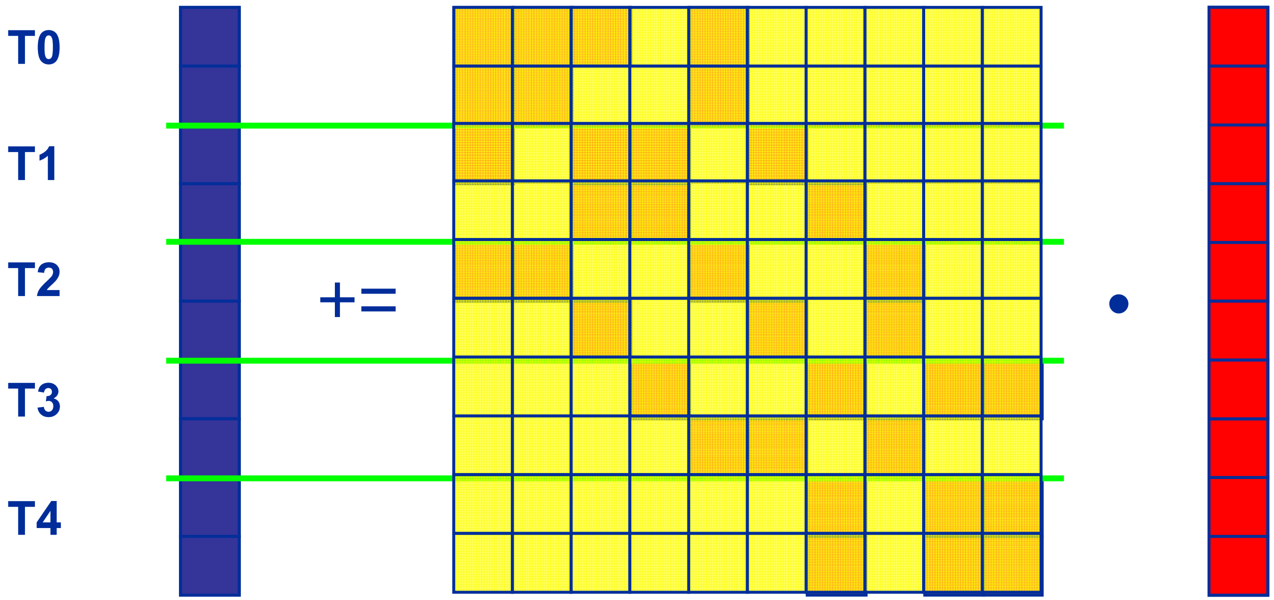
Common OpenMP pitfalls

- Correctness
  - Deadlock: Thread waits for resources that never become available
    - Write correct programs (tools help to detect deadlocks)
  - Race condition: Uncontrolled writes to shared variable
    - Use `private` clause
- Performance
  - False sharing: Frequent writes from different threads to same cache line
    - Insert padding, choose appropriate OpenMP schedule
  - Load imbalance: Different workloads assigned to different threads leads to idling CPUs
    - Use dynamic or guided schedule, rearrange workload
  - OpenMP loop overhead: Loop is too short to amortize the cost of starting a team of threads
    - Use programming techniques to fatten loop body

OpenMP parallelization of sparse MVM

Data parallelism for sparse MVM

- Parallelize the loop that treats consecutive elements of result vector (or consecutive matrix rows)
- General idea:



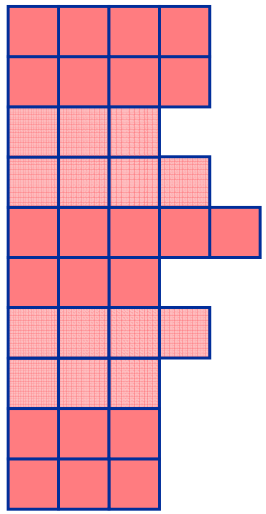
- RHS vector is accessed by all threads
  - … but this is shared memory, so it does not have to be stored multiple times!

OpenMP parallelization of CRS MVM

- Parallelized loop is outer loop

```
!$OMP parallel do
do i = 1,Nr
 do j = row_ptr(i), row_ptr(i+1) - 1
  c(i) = c(i) + val(j) * b(col_idx(j))
 enddo
enddo
!$OMP end parallel do
```

- Features
  - Long outer loop
    - small OpenMP overhead
  - Variable length of inner loop
    - possible load imbalance



OpenMP parallelization of JDS MVM

- Parallelized loop is inner loop

```
!$OMP parallel private(diag,diagLen,offset,i)
do diag=1, zmax
  diagLen = jd_ptr(diag+1) - jd_ptr(diag)
  offset  = jd_ptr(diag)
!$OMP do
  do i=1, diagLen
    c(i) = c(i) + val(offset+i) * b(col_idx(offset+i))
  enddo
!$OMP end do
enddo
!$OMP end parallel
```

- Features
  - Long inner loop
  - No load imbalance problems

OpenMP parallelization of blocked JDS MVM

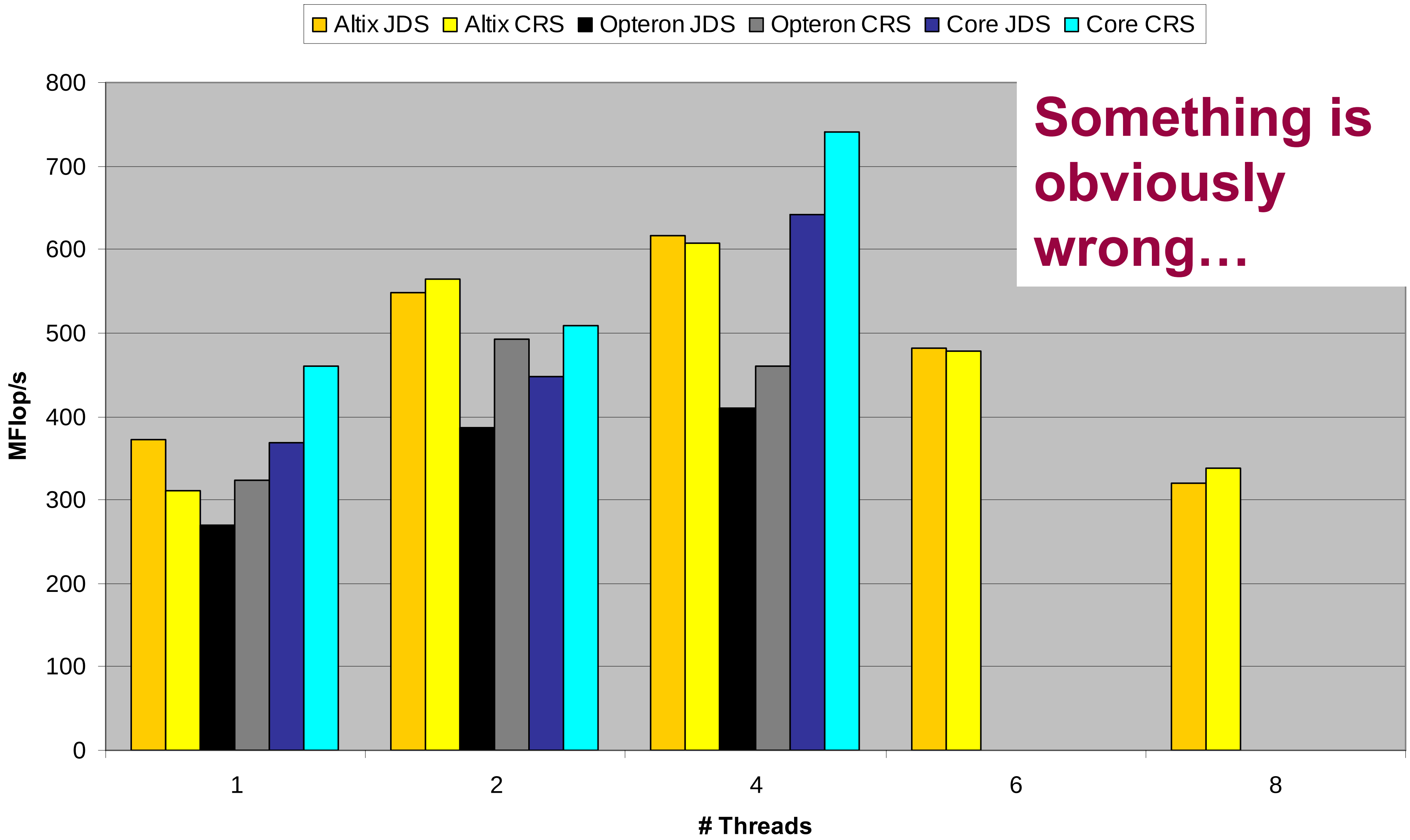
- Parallelization can now be pulled to outer loop

```
!$OMP parallel do private(block_start,block_end,i,diag,
!$OMP& diagLen,offset)
do ib=1, maxDiagLen, blocklen
  block_start = ib
  block_end   = min(ib+blocklen-1, maxDiagLen)
  do diag=1, zmax
    diagLen = jd_ptr(diag+1)-jd_ptr(diag)
    offset  = jd_ptr(diag)
    if(diagLen .ge. block_start) then
      do i=block_start, min(block_end,diagLen)
        c(i) = c(i)+val(offset+i)*b(col_idx(offset+i))
      enddo
    endif
  enddo
enddo
!$OMP end parallel do
```

- Features
  - Least OpenMP overhead
  - Some load imbalance possible

Parallel sparse MVM: Scalability

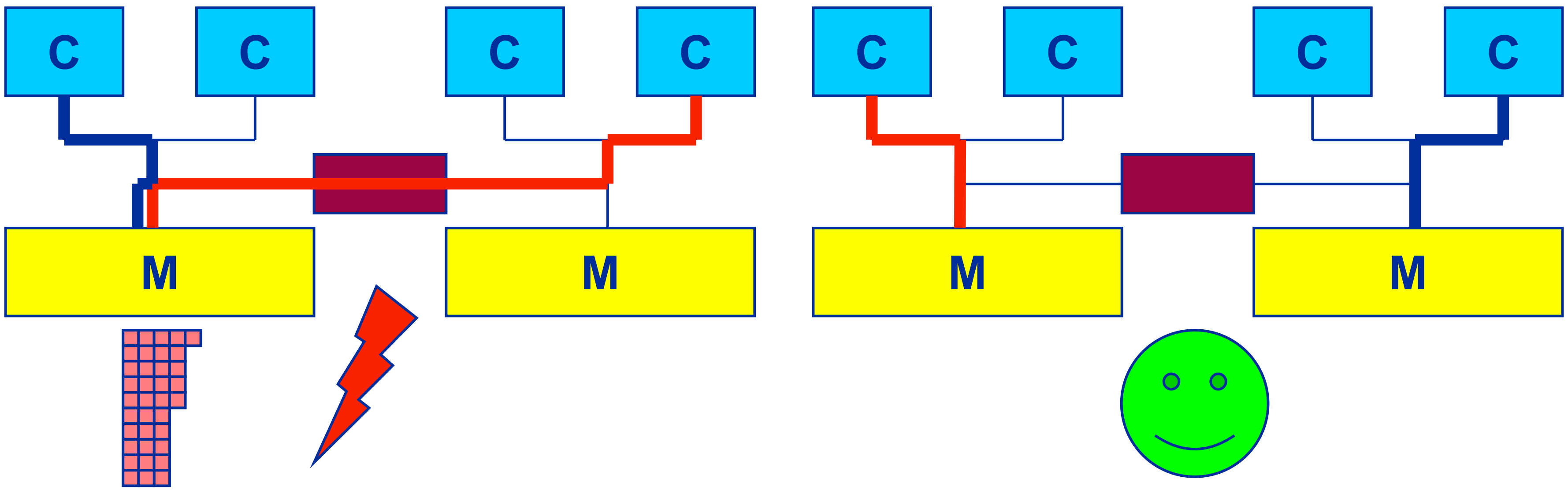
- **Scalability data for OpenMP version**



Data locality in ccNUMA systems

Memory Locality Problems

- **ccNUMA:**
  - **whole memory is transparently accessible by all processors**
  - **but physically distributed**
  - **with varying bandwidth and latency**
  - **and potential congestion (shared memory paths)**
- **How do we make sure that memory access is always as "local" and "distributed" as possible?**



Coding for Data Locality

- **In OpenMP the programmer must ensure that memory pages**
  - **get mapped locally, i.e. data that is accessed from CPU n should reside in a local memory block**
  - **rigorously apply the "Golden Rule":**

    A <u>memory page</u> gets mapped into the local memory of the processor that first touches (reads or writes to) it!

- **i.e. we have to take a closer look at initialization code**

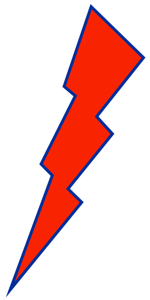
- **Locality is always observed on the page level**
  - **Page sizes: 4kB, 16kB, sometimes larger**

- **Some false (page) sharing at domain boundaries may be unavoidable**

Coding for Data Locality

- **Simplest case: explicit initialization**

```
Integer,parameter :: N=1000000
Real*8 A(N), B(N)

A=0.d0

!$OMP parallel do
Do I = 1, N
   B(i) = function ( A(i) )
End do
```

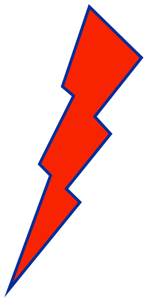


```
Integer,parameter :: N=1000000
Real*8 A(N),B(N)

!$OMP parallel do
Do I = 1, N
   A(i)=0.d0
End do

!$OMP parallel do
Do I = 1, N
   B(i) = function ( A(i) )
End do
```

Coding for Data Locality

- **Sometimes initialization is not so obvious: I/O cannot be easily parallelized, so "localize" arrays before I/O**

```
Integer,parameter :: N=1000000
Real*8 A(N), B(N)

READ(1000) A
!$OMP parallel do
Do I = 1, N
   B(i) = function ( A(i) )
End do
```



```
Integer,parameter :: N=1000000
Real*8 A(N),B(N)

!$OMP parallel do
Do I = 1, N
   A(i)=0.d0
End do
READ(1000) A
!$OMP parallel do
Do I = 1, N
   B(i) = function ( A(i) )
End do
```

Coding for Data Locality

- Required condition: OpenMP loop schedule of initialization must be the same as in all computational loops
  - best choice: `static`! Specify explicitly on all NUMA-sensitive loops, just to be sure…
  - imposes some constraints on possible optimizations (e.g. load balancing) → some sensibly large chunk size may be better than plain `static`

- How about global objects?
  - better not use them
  - if communication vs. computation is favorable, might consider properly placed copies of global data
  - in C++, STL allocators provide an elegant solution

Data locality in parallel sparse MVM

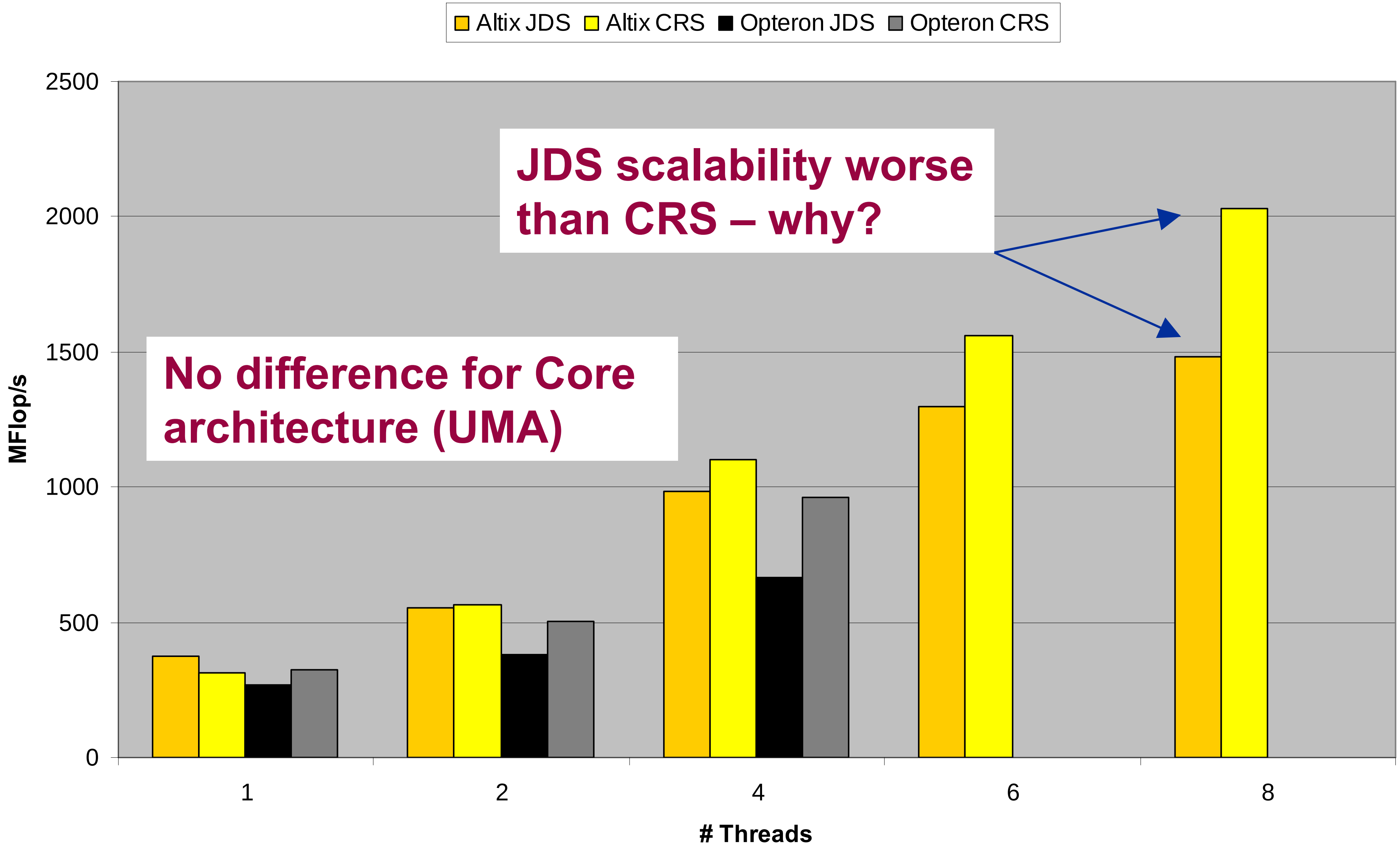
- No code change in MVM loop required (apart from static schedule)
- CRS
  - Initialization of arrays val[], c[], b[], row_ptr[] and col_idx[] must be done in parallel

```
!$OMP parallel do private(start,end,j)
!$OMP& schedule(static)
do i=1,Nr
  start = row_ptr(i)
  end = row_ptr(i+1)
  do j=start,end-1
    val(j) = 0.d0
    col_idx(j)= 0
  enddo
enddo
```

- Similar for JDS

Parallel sparse MVM
Doing it right on ccNUMA

- **Correct placement leads to acceptable scalability**



- **Bck to C++: Don't forget that constructors tend to touch the data members of an object. Example:**

```
class D {
  double d;
public:
  D(double _d=0.0) throw() : d(_d) {}
  inline D operator+(const D& o) throw() {
    return D(d+o.d);
  }
  inline D operator*(const D& o) throw() {
    return D(d*o.d);
  }
...
};
```

→ **placement problem with**

```
D* array = new D[1000000];
```

Coding for Data Locality: C++ issues

- **Solution: Provide overloaded new operator or special function that places the memory before constructors are called (PAGE_BITS = base-2 log of pagesize)**

```
template <class T> T* pnew(size_t n) {
  size_t st = sizeof(T);
  int ofs,len=n*st;
  int i,pages = len >> PAGE_BITS;
  char *p = new char[len];
#pragma omp parallel for schedule(static) private(ofs)
    for(i=0; i<pages; ++i) {
      ofs = static_cast<size_t>(i) << PAGE_BITS;
      p[ofs]=0;
    }
#pragma omp parallel for schedule(static) private(ofs)
    for(ofs=0; ofs<n; ++ofs) {
      new(static_cast<void*>(p+ofs*st)) T;
    }
  return static_cast<T*>(m);
}
```

parallel first touch

placement new!

Coding for Data Locality: NUMA allocator for parallel first touch

```
template <class T> class NUMA_Allocator {
public:
  T* allocate(size_type numObjects, const void
                *localityHint=0) {
    size_type ofs,len = numObjects * sizeof(T);
    void *m = malloc(len);
    char *p = static_cast<char*>(m);
    int i,pages = len >> PAGE_BITS;
#pragma omp parallel for schedule(static) private(ofs)
    for(i=0; i<pages; ++i) {
      ofs = static_cast<size_t>(i) << PAGE_BITS;
      p[ofs]=0;
    }
    return static_cast<pointer>(m);
  }
...
};
```

Application:

```
vector<double,NUMA_Allocator<double> > x(1000000)
```

References

- OpenMP Home: Specifications, resources, mailing list, events
  http://www.openmp.org/
- G. Hager, T. Zeiser, J. Treibig and G. Wellein:
  Optimizing performance on modern HPC systems: learning from simple kernel benchmarks.
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BACKUP

Application: DMRG – Parallelization of sparse MVM in superblock diagonalization

- **Sparse MVM: Sum over dense matrix-matrix multiplies!**

$$\sum_{i'j'} H_{ij;i'j'}\psi_{i'j'} = \sum_{\alpha}\sum_{i'} A^{\alpha}_{ii'} \sum_{j'} B^{\alpha}_{jj'}\psi_{i'j'}$$

- **However, *A* and *B* may contain only a few nonzero elements, e.g. if conservation laws (quantum numbers) have to be obeyed**
- **To minimize overhead an additional loop (running over nonzero blocks only) is introduced**

$$H\psi = \sum_{\alpha}\sum_{k} (H\psi)^{\alpha}_{L(k)} = \sum_{\alpha}\sum_{k} A^{\alpha}_{k}\psi_{R(k)}\left[B^{\mathrm{T}}\right]^{\alpha}_{k}$$

Sparse MVM in DMRG

Implementation of sparse MVM - pseudocode

$$H\psi = \sum_{\alpha} \sum_{k} A_k^{\alpha} \psi_{R(k)} \left[B^{\mathrm{T}}\right]_k^{\alpha}$$

```
// W: wavevector ; R: result
for (α=0; α < number_of_hamiltonian_terms; α++) {

        term = hamiltonian_terms[α];

        for (k=0 ; k < term.number_of_blocks; k++) {

                li = term[k].left_index;
                ri = term[k].right_index;

                temp_matrix = term[k].B.transpose() * W[ri];

                R[li] += term[k].A * temp_matrix;

        }}
```

Parallel loop !? (outer loop over α)

Parallel loop !? (inner loop over k)

Matrix-matrix multiply (arrows to `term[k].B.transpose() * W[ri]` and `term[k].A * temp_matrix`)

Data dependency ! (arrow to `R[li]`)

DMRG: OpenMP Parallelization

- **Parallelization of innermost k loop: Scales badly**
  - **loop too short**
  - **collective thread operations within outer loop**
- **Parallelization of outer α loop: Scales badly**
  - **even shorter**
  - **load imbalance (trip count of k loop depends on α)**

- **Solution:**
  - **"Fuse" both loops (α & k)**
  - **Protect write operation `R[li]` with lock mechanism**
  - **Use list of OpenMP locks for each block `li`**

DMRG: OpenMP Parallelization

Preparation

```
// store all block references in block_array
ics=0;
for (α=0; α < number_of_hamiltonian_terms; α++) {
        term = hamiltonian_terms[α];
        for (k=0 ; k < term.number_of_blocks; k++) {
                block_array[ics]=&term[q];
                ics++;
        }}
icsmax=ics;


// set up lock lists
for(i=0; i < MAX_NUMBER_OF_THREADS; i++)
        mm[i] = new Matrix // temp.matrix

for (i=0; I < MAX_NUMBER_OF_LOCKS; i++) {
        locks[i]= new omp_lock_t;
        omp_init_lock(locks[i]);
        }
```

DMRG: OpenMP Parallelization

```
// W: wavevector ; R: result
#pragma omp parallel private(mymat, li, ri, myid, ics)
{
        myid = omp_get_thread_num();
        mytmat = mm[myid]; // temp thread local matrix

#pragma omp for
        for (ics=0; ics< icsmax; ics++) {

        li = block_array[ics]->left_index;
        ri = block_array[ics]->right_index;

        mytmat = block_array[ics]->B.transpose() * W[ri];

        omp_set_lock(locks[li]);
        R[li] += block_array[ics]->A * mytmat;
        omp_unset_lock(locks[li]);
        }
}
```

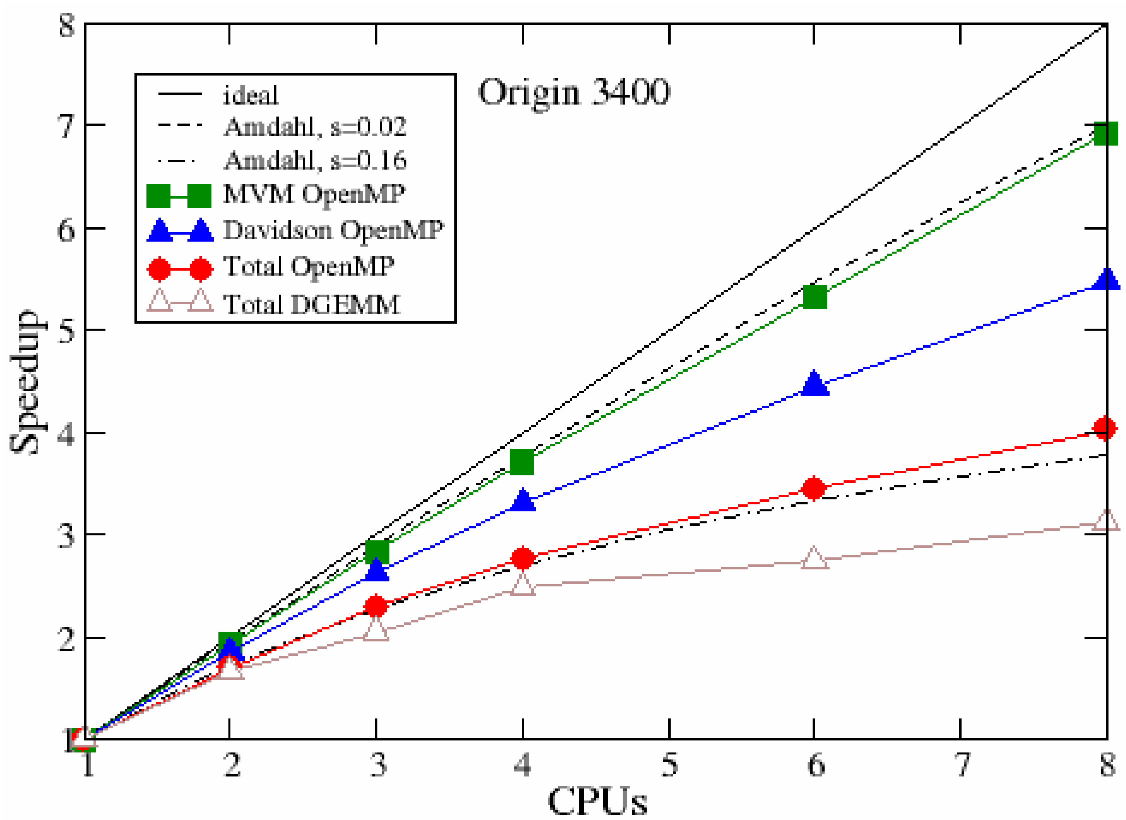
Fused (α,k) loop

Protect each block of result vector **R** with locks

DMRG : OpenMP Parallelization

Scalability on SGI Origin

- **`OMP_SCHEDULE=STATIC`**
- **OpenMP scales significantly better than parallel DGEMM**
- **Serial overhead in parallel MVM is only about 5%**



DMRG : OpenMP Parallelization
Further improvements

- **Chose best distribution strategy for parallel for loop:**
  `OMP_SCHEDULE="dynamic,2"`
  (reduces serial overhead in MVM to 2%)

- **Re-link with parallel LAPACK/BLAS to speed up density-matrix diagonalization (DSYEV)**
  - **Observe vendor advice**