Parallel Computing
Introduction and Shared Memory Programming

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Outline

- Part 1
  - Introduction, motivation
  - Understanding parallelism
  - Limitations of parallelism

- Part 2
  - Shared Memory architectures
  - Some comments about multi-core
  - Cache coherence
  - Introduction to OpenMP as an example for shared memory programming
  - Programming guidelines for ccNUMA architecture
**Introduction**

**Parallel Computing**

- Parallelism will substantially increase through the use of dual/multi-core chips in the future!
  - See later for some comments

- Parallel computing is entering everyday life
  - Dual-core based system (Workstation, Laptop, etc…)

- Basic design concepts for parallel computers:
  - **Shared memory multi-processor systems**: Multiple processors run in parallel but use the same (a single) address space ("shared memory"), e.g.: Dual-core workstations or Xeon/Opteron based servers.

  - **Distributed memory systems**: Multiple processors/compute nodes are connected via a network. Each processor has its own address space/memory, e.g. GBit Clusters with Xeon/Opteron based servers.

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**Understanding Parallelism and the Limitations of Parallel Computing**
Understanding Parallelism:

Sequential work

After 16 time steps: 4 cars

Parallel work

After 4 time steps: 4 cars

“perfect speedup”
Understanding Parallelism:
Limits of Scalability

Unused resources due to load imbalance

Limitations of Parallel Computing:
Amdahl's Law

Ideal world:
All work is perfectly parallelizable

Closer to reality:
Purely serial parts limit maximum speedup

Reality is even worse:
Communication processes hurt scalability even further
Limitations of Parallel Computing:
Calculating Speedup in a Simple Model ("strong scaling")

- $T(1) = s + p = \text{serial compute time}$
- Parallelizable part: $p = 1 - s$
- Purely serial part $s$
- General formula for speedup (worst case):
  \[ S^k_p = \frac{T(1)}{T(N)} = \frac{1}{s + \frac{1-s}{N} + Nk} \]

Limitations of Parallel Computing:
Amdahl's Law ("strong scaling")

- Reality: No task is perfectly parallelizable
  - Shared resources have to be used serially
  - Task interdependencies must be accounted for
  - Communication overhead
- Benefit of parallelization is strongly limited
  - "Side effect": limited scalability leads to inefficient use of resources
  - Metric: Parallel Efficiency
    (what percentage of the workers/processors is efficiently used):
    \[ \varepsilon_p(N) = \frac{S_p(N)}{N} \]
- Amdahl case:
  \[ \varepsilon_p = \frac{1}{s(N-1)+1} \]
Limitations of Parallel Computing: Amdahl’s Law (“strong scaling”)

- Large N limits
  - at k=0, Amdahl’s Law predicts
    \[ \lim_{N \to \infty} S_p^0(N) = \frac{1}{s} \]
    independent of N!
  - at k≠0, our simplified model of communication overhead yields a behaviour of
    \[ S_p^k(N) \xrightarrow{N \to \infty} \frac{1}{Nk} \]

- Problems in real world programming
  - Load imbalance
  - Shared resources have to be used serially (e.g. IO)
  - Task interdependencies must be accounted for
  - Communication overhead

![Graph showing Amdahl's Law](image-url)
Limitations of Parallel Computing:

Amdahl’s Law (“strong scaling”)

Parallel efficiency:

- <10%
- ~50%

\[
S(N) = \frac{1}{s + \frac{k}{N}}
\]

- \(s=0.01\)
- \(s=0.1\)
- \(s=0.1, k=0.05\)

# CPUs

S(N)

Communication is not necessarily purely serial

- Non-blocking crossbar networks can transfer many messages concurrently – factor \(Nk\) in denominator becomes \(k\) (technical measure)
- Sometimes, communication can be overlapped with useful work (implementation, algorithm):

Communication overhead may scale with a smaller power than problem size

"superlinear speedups": data size per CPU decreases with increasing CPU count \(\Rightarrow\) may fit into cache at large CPU counts
Limitations of Parallel Computing:
Increasing Parallel Efficiency

- Increasing problem size often helps to enlarge the parallel fraction \( p \)
  - Often \( p \) scales with problem size while \( s \) stays constant
  - Fraction of \( s \) relative to overall runtime decreases

\[
\text{Scalability in terms of parallel speedup and parallel efficiency}
\text{improves when scaling the problem size!}
\]

Limitations of Parallel Computing:
Increasing Parallel Efficiency ("weak scaling")

- When scaling a problem to more workers, the amount of work will often be scaled as well
  - Let \( s \) and \( p \) be the serial and parallel fractions so that \( s + p = 1 \)
  - Perfect situation: runtime stays constant while \( N \) increases
  - "Parallel Performance" =

\[
P_i(N) = \frac{s + pN}{s + p} = s + pN = N + (1 - N)s = s + (1 - s)N
\]

Gustafsson's Law
("weak scaling")

- Linear in \( N \) – but closely observe the meaning of the word "work"!

\[
\text{work/time for problem size } N \text{ with } N \text{ workers}
\]

\[
\text{work/time for problem size 1 with 1 worker}
\]

\[
P_i(N) = \frac{s + pN}{s + p} = s + pN = N + (1 - N)s = s + (1 - s)N
\]
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

Shared memory computers:
ccNUMA

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 2” node
- Dual AMD Opteron node
- SGI Altix (HLRB2 @ LRZ)

Shared memory computers
Cache coherence

- 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**
  - Load A1
  - Write A1=0

  **P2**
  - Load A2
  - Write A2=0

  Write-back to memory leads to incoherent data

  A1, A2

  C1 & C2 entry can not be merged to:

  A1, A2
Cache coherence protocol must keep track of cache line (CL) status.

**Cache Coherence Diagram**

- **P1**
  - Load A1
  - Write A1=0:
    1. Request exclusive access to CL
    2. Invalidate CL in C2
    3. Modify A1 in C1

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

**C2 is exclusive owner of CL**

- **A1, A2**
- **Memory**
- **Bus**

---

**Cache Coherence**

- **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")!
Why Multi-Core?

- Modern processors are highly complex
- With each new generation, more transistors are required to achieve a certain performance gain
  - Even highly optimized software leaves more and more transistors unused
- All those transistors need energy (switching/leakage)
Power dissipation in VLSI Circuits

- In CMOS VLSIs, power dissipation is proportional to clock frequency:
  \[ W \propto f_c \]

- Moreover, it is proportional to supply voltage squared:
  \[ W \propto V_{cc}^2 \]

- For reasons of noise immunity, supply voltage has to grow linearly with frequency, so:
  \[ W \propto f_c^3 \]

- Frequency reduction is the key to saving power with modern microprocessors
  - all other factors, e.g. manufacturing technology, unchanged
  - This seems to contradict the verdict of ever-growing chip performance

Multi-core processors

*The party is over!*

- **Problem:** Moore’s law is still valid but increasing clock speed hits a technical wall (heat)
- **Solution:** Reduce clock speed of processor but put 2 (or more) processors (cores) on a single silicon die
  
  **Clock speed of single core will decrease in future!**
  
  (Xeon/Netburst: max. 3.73 GHz –> Xeon/Core: max. 3.0 GHz)

![Multi-core processors diagram](image-url)
Multi-core processors
The party is over!

By courtesy of D. Vrsalovic, Intel

Over-clocking (+20%)

1.13x

1.73x

Performance
Power

1.00x

Max Frequency

1.00x

Performance
Power

Multi-core processors
The party is over!

By courtesy of D. Vrsalovic, Intel
Multi-core processors

The party is over!

By courtesy of D. Vrsalovic, Intel

[Bar chart showing performance, power, and frequency comparisons for over-clocked and under-clocked Dual-Core and Multi-core processors]

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Multi-Core Processors

- **Question:** What fraction of performance must be sacrificed per core in order to benefit from $m$ cores?
- **Prerequisite:** Overall power dissipation should be unchanged

- $W$ power dissipation
- $p$ performance (1 core)
- $p_m$ performance ($m$ cores)
- $\varepsilon_f$ rel. frequency change $f_m/f_c$
- $\varepsilon_p$ rel. performance change $p_m/p$
- $m$ number of cores

\[
W + \Delta W = (1 + \varepsilon_f)^3 W
\]

\[
(1 + \varepsilon_f)^3 m = 1
\]

\[
\varepsilon_f = m^{-1/3} - 1
\]

\[
p_m = (1 + \varepsilon_p) p_m
\]

\[
p_m \geq p \Rightarrow \varepsilon_p \geq \frac{1}{m} - 1
\]

Why Multi-Core?

- **Required relative frequency reduction vs. core count**

Available today
Multi-core processors

A challenging future ahead?

Parallelization will be mandatory in the future!

Multi-core processors

A challenging future ahead?

Multi-Core

A Challenging Future or the Programmer’s Waterloo?

- Multi-core does not come for free
  - i.e., frequency reduction is not enough
- Putting two cores on the same die requires either
  - changes in manufacturing technology (smaller structures), or
  - simplification of the core
- Moore’s Law is still valid, so multi-core must put the transistors to good use
  - Simplify the core (better utilization of functional units)
  - Increase the cache sizes using the saved transistors
- Are we giving up the “general-purpose“ processor for more and more specialized solutions?
- Caveat: While multi-core enhances chip performance, it makes the DRAM gap more severe
  - Shared path to memory
Shared-Memory Parallelization with OpenMP

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 written to compile and execute on a single-processor machine just by ignoring the directives
  - API calls must be masked out though
  - Supports data parallelism
**Shared Memory Model used by OpenMP**

- **Central concept of OpenMP programming: Threads**
  - 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
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

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

\[ \rightarrow \text{solve this in OpenMP} \]

program compute_pi

... (declarations omitted)

! function to integrate

\[ f(a) = \frac{4.0_8}{(1.0_8 + a^2)} \]

\[ w = \frac{1.0_8}{n} \]

\[ \text{sum} = 0.0_8 \]

do i=1,n

\[ x = w * (i-0.5_8) \]

\[ \text{sum} = \text{sum} + f(x) \]

enddo

\[ \text{pi} = w * \text{sum} \]

... (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 

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)
OpenMP Directives
Syntax in C/C++

- 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
  ...
  #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 (static in C)
  2. Loop variables of parallel ("sliced") loops are private

- Due to stack size limits it may be necessary to make large arrays static
  - 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)
  ```

- 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

Compiling and running an OpenMP program

- Compiler must be instructed to recognize OpenMP directives (Intel compiler: `-openmp`)

- 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

- ... and then: just type `.a.out`
Some Details About OpenMP

OpenMP Runtime Library

- **omp_get_num_threads** Function
  Returns the number of threads currently in the team executing the parallel region from which it is called
  - Fortran:
    ```
    integer function omp_get_num_threads()
    ```
  - C/C++:
    ```
    int omp_get_num_threads(void);
    ```

- **omp_get_thread_num** Function
  Returns the thread number, within the team, that lies between 0 and `omp_get_num_threads() - 1`, inclusive. The master thread of the team is thread 0
  - Fortran:
    ```
    integer function omp_get_thread_num()
    ```
  - C/C++:
    ```
    int omp_get_thread_num(void);
    ```
OpenMP Example: Hello World Program

program hello
  !$ integer OMP_GET_THREAD_NUM
  i = -1
  !$OMP PARALLEL PRIVATE(i)
  !$ i = OMP_GET_THREAD_NUM()
  print *, 'hello world', i
  !$OMP END PARALLEL
  stop
end

Work Sharing and Synchronization

- Which thread executes which statement or operation?
  - ... and in which sequence?

- i.e., how is parallel work organized/scheduled?
  - Work-sharing constructs
  - Master and synchronization constructs
OpenMP Work Sharing Constructs

- Distribute the execution of the enclosed code region among the members of the team
  - Must be enclosed dynamically within a parallel region
  - Threads do not (usually) launch new threads
  - No implied barrier on entry

- Directives
  - section(s) directives
  - do directive (Fortran)
  - for directive (C/C++)

OpenMP sections Directives (1)

- Several blocks are executed in parallel
  - Fortran:
    - !$OMP SECTIONS [ clause[ , , ] clause ] ... ]
    - !$OMP SECTION
      - block1
    - !$OMP SECTION
      - block2
    ...
    - !$OMP END SECTIONS [ nowait ]
  - C/C++:
    - #pragma omp sections [ clause [ clause ] ... ] new-line
      {  
        [ #pragma omp section new-line ]
        structured-block1
        [ #pragma omp section new-line ]
        structured-block2
        ...
      }

OpenMP sections Directives (2)

C/C++:
```
#pragma omp parallel
{
#pragma omp sections
{{
 a=...;
 b=...;
}
#pragma omp section
{ c=...;
 d=...;
}
#pragma omp section
{ e=...;
 f=...;
}
#pragma omp section
{ g=...;
 h=...;
}
} /*omp end sections*/
} /*omp end parallel*/
```

OpenMP do/for Directives (1)

- Immediately following loop is executed in parallel
- Fortran:
  ```
  !$OMP do [ clause [ , ] clause ] ...
  do_loop
  [ !$OMP end do [ nowait ] ]
  ```
- If used, the `end do` directive must appear immediately after the end of the loop
- C/C++:
  ```
  #pragma omp for [ clause [ clause ] ... ] new-line
  for-loop
  ```
- The corresponding `for` loop must have "canonical shape":
  ```
  for (i=start; i<=end; i++) { ... }
  ```
OpenMP do/for Directives (2)

C/C++:

```c
#pragma omp parallel private(f)
{
    f=7;
    #pragma omp for
    for (i=0; i<20; i++)
        a[i] = b[i] + f * (i+1);
} /* omp end parallel */
```

OpenMP do/for Directives (3)

- `clause` can be one of the following:
  - `private(list)` [see later: Data Model]
  - `reduction(operator:list)` [see later: Data Model]
  - `schedule(type [, chunk])`
  - `nowait` (C/C++: on #pragma omp for) (Fortran: on $!OMP END DO)
  - ...

- Implicit barrier at the end of do/for unless `nowait` is specified
- If `nowait` is specified, threads do not synchronize at the end of the parallel loop
- `schedule` clause specifies how iterations of the loop are distributed among the threads of the team.
  - Default is implementation-dependent
OpenMP schedule Clause

Within `schedule(type[, chunk])` type can be one of the following:

- **static**: Iterations are divided into pieces of a size specified by `chunk`. The pieces are statically assigned to threads in the team in a round-robin fashion in the order of the thread number.  
  *Default chunk size: one contiguous piece for each thread.*

- **dynamic**: Iterations are broken into pieces of a size specified by `chunk`. As each thread finishes a piece of the iteration space, it dynamically obtains the next set of iterations.  
  *Default chunk size: 1.*

- **guided**: The chunk size is reduced in an exponentially decreasing manner with each dispatched piece of the iteration space.  
  *chunk specifies the smallest piece (except possibly the last).*  
  *Default chunk size: 1.*  
  *Initial chunk size is implementation dependent.*

- **runtime**: The decision regarding scheduling is deferred until run time. The schedule type and chunk size can be chosen at run time by setting the `OMP_SCHEDULE` environment variable.  
  *Default schedule: implementation dependent.*

Loop scheduling

```
static  dynamic(3)  guided(1)
```

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Dense matrix vector multiplication

start_time = ...
!$OMP PARALLEL PRIVATE(N,J,I)
do n = 1 , loops
!$OMP DO SCHEDULE(RUNTIME)
do i=1,N
   do j=1,N
      y(i)=y(i)+a(j,i)*x(j)
   end do
end do
!$OMP END DO
   call obscure(…) ! Do not interchange n & (i,j) loops
enddo
!$OMP END PARALLEL
end_time = ...

\[\text{SCHEDULE=STATIC,1} \quad \text{SCHEDULE=STATIC,8} \quad \text{SCHEDULE=STATIC,16}\]
Dense matrix vector multiplication

SGI Origin; OMP_NUM_THREADS = 4

SCHEDULE=STATIC
SCHEDULE=DYNAMIC,1
SCHEDULE=DYNAMIC,16
SCHEDULE=GUIDED,1
SCHEDULE=GUIDED,8
Dense matrix vector multiplication
SGI Origin; OMP SCHEDULE=STATIC

Dense Matrix-Vector-Multiply
Outer-Loop-Parallel; SCHEDULE=STATIC; SGI O3K

OMP_NUM_THREADS=1
OMP_NUM_THREADS=2
OMP_NUM_THREADS=4
OMP_NUM_THREADS=8
OMP_NUM_THREADS=16

MFlop/s per processor

N
0 500 1000 1500 2000
0 100 200 300 400 500

Dense matrix vector multiplication
SGI Origin; OMP SCHEDULE=STATIC

Dense Matrix-Vector-Multiply
Outer-Loop-Parallel; SCHEDULE=STATIC; SGI O3K

OMP_NUM_THREADS=1
OMP_NUM_THREADS=2
OMP_NUM_THREADS=4
OMP_NUM_THREADS=8
OMP_NUM_THREADS=16

MFlop/s

N
0 500 1000 1500 2000
0 100 200 300 400 500
Conditional parallelism: if clause

- Allows execution of a code region in serial or parallel, depending on a condition

- Fortran:
  ```
  !$omp parallel if (condition)
  ... (block)
  !$omp end parallel
  ```

- C/C++:
  ```
  #pragma omp parallel if(condition)
  
  ```

- Usage:
  - disable parallelism dynamically
  - define crossover points for optimal performance
  - may require manual or semi-automatic tuning

Example for crossover points:
Vector triad with 4 threads on 4-CPU Itanium2
OpenMP reduction Clause

- reduction (operator: list)
- Performs a reduction on the variables that appear in list, with the operator operator
- operator: one of
  - Fortran:
    +, *, -, .and., .or., .eqv., .neqv., or
    max, min, iand, ior, or ieor
  - C/C++:
    +, *, -, &, ^, |, &&, or ||
- Variables must be shared in the enclosing context
- At the end of the reduction, the shared variable is updated to reflect the result of combining the original value of the shared reduction variable with the final value of each of the private copies using the operator specified

OpenMP reduction — an example (C/C++)

C / C++:

```c
sm = 0;
#pragma parallel
{
#pragma omp for private(r)
   reduction(+:sm)
   for( i=0; i<20; i++)
   { r = work(i);
     sm = sm + r;
   }
   /*end for*/
} /*end parallel*/
printf("sum=%f\n",sm);
```
Example: Solving the heat conduction equation

- **Square piece of metal**
  - Temperature \( \Phi(x,y,t) \)
  - Boundary values:
    \( \Phi(x,1,t) = 1, \quad \Phi(x,0,t) = 0, \quad \Phi(0,y,t) = y = \Phi(1,y,t) \)
  - Initial values for all \( x, y < 1 \) are zero

- **Temporal evolution**:
  - to stationary state
  - partial differential equation

\[
\frac{\partial \Phi}{\partial t} = \frac{\partial^2 \Phi}{\partial x^2} + \frac{\partial^2 \Phi}{\partial y^2}
\]

Heat conduction (2): algorithm for solution

- **Interested in stationary state**
  - discretization in space: \( x_i, y_i \)
    \( \rightarrow \) 2-D Array \( \Phi \)
  - discretization in time:
    \( \rightarrow \) steps \( \Delta t \)

Repeatedly calculate increments

\[
\delta \Phi(i,k) = \Delta t \left[ \frac{\Phi(i+1,k) + \Phi(i-1,k) - 2\Phi(i,k)}{dx^2} + \frac{\Phi(i,k+1) + \Phi(i,k-1) - 2\Phi(i,k)}{dy^2} \right]
\]

until \( \delta \Phi = 0 \) reached.
Heat Conduction (3): data structures

- 2-dimensional array \( \phi \) for heat values
- equally large \( \phi_{\text{in}} \), to which updates are written
- Iterate updates until stationary value is reached
- Both arrays shared
- Tile grid area to OpenMP threads

Heat Conduction (3): code for updates

```
! iteration  
do it=1,itmax  
dphimax=0.  
!$OMP parallel do private(dphi,i) reduction(max:dphimax)  
do k=1,kmax-1  
do i=1,imax-1  
dphi=(phi(i+1,k)+phi(i-1,k)-2.0_8*phi(i,k))*dy2i  &  
   +(phi(i,k+1)+phi(i,k-1)-2.0_8*phi(i,k))*dx2i  
dphi=dphi*dt  
dphimax=max(dphimax,abs(dphi))  
phin(i,k)=phi(i,k)+dphi  
enddo  
enddo  
!$OMP end parallel do  

!$OMP parallel do  
do k=1,kmax-1  
do i=1,imax-1  
phi(i,k)=phin(i,k)  
enddo  
enddo  
!$OMP end parallel do  

!required precision reached?  
if(dphimax.lt.eps) goto 10  
enddo  
10 continue
```
OpenMP Synchronization

- **Implicit Barrier**
  - beginning and end of `parallel` constructs
  - end of all other control constructs
  - implicit synchronization can be removed with `nowait` clause

- **Explicit synchronization**
  - `critical`
  - `atomic`
  - `single`
  - `master`
  - `barrier`
  - `flush`
  - `omp_set_lock()` and similar API functions

Synchronization Constructs: 
**single** directive

- The enclosed code is executed by exactly one thread, which one is unspecified

- **Fortran:**
  ```
  !$OMP SINGLE [clause[,]clause]... block
  !$OMP END SINGLE [NOWAIT]
  ```

- **C/C++:**
  ```
  #pragma omp single [clause[,]clause]... [nowait] new-line structured-block
  ```
### Synchronization Constructs: single directive

- The other threads in the team skip the enclosed section of code and continue execution. There is an implied barrier at the exit of the single section!
- may not appear within a parallel do (deadlock!)
- `nowait` clause after `end single` (or at start of parallel region in C/C++) suppresses synchronization

### Synchronization Constructs: barrier directive

- Synchronizes all threads in the team
- **Fortran:**
  ```fortran
  !$OMP BARRIER
  ```
- **C/C++:**
  ```c
  #pragma omp barrier
  ```
  In C(++) the directive must appear inside a block or compound statement
- After all threads have encountered the barrier, they continue to execute the code after it in parallel
- **Barrier is a collective operation:** it must either be encountered by all threads in the team or none at all
  - else: deadlock!
Synchronization Constructs:
API Locking Functions

- OpenMP API provides some functions that allow explicit locking (POSIX: "mutex")
- Explicit locking has user-defined semantics
  - The compiler knows nothing about the binding of a lock to a resource
- Simple variables can be protected by directives (atomic/critical), but how about more complicated constructs?
  - User-defined data structures
  - Thread-unsafe library routines
  - Arrays of objects
  - …
- API functions allow more flexible strategies when a resource is locked
  - Lock may be tested without blocking

API Locking Functions

Threads must agree on which lock protects which resource!
API Locking Functions:

**Lock Definitions**

- A lock must be defined and initialized before it can be used
  - **Fortran:**
    ```fortran
    INTEGER (KIND=OMP_LOCK_KIND) :: lockvar
    CALL OMP_INIT_LOCK(lockvar)
    ```
  - **C/C++:**
    ```c
    #include <omp.h>
    omp_lock_t lockvar;
    omp_init_lock(&lockvar);
    ```
- Initialization is required to use the lock afterwards
- Lock can be removed (uninitialized) if not needed any more
  - **OMP_DESTROY_LOCK** subroutine, `omp_destroy_lock()` function

**Setting and Unsetting Locks**

- Setting and unsetting a lock is an **atomic** operation
  - **Fortran:**
    ```fortran
    CALL MP_SET_LOCK(lockvar)
    CALL MP_UNSET_LOCK(lockvar)
    ```
  - **C/C++:**
    ```c
    omp_set_lock(&lockvar);
    omp_unset_lock(&lockvar);
    ```
- `lockvar` must be an initialized lock variable
- Setting the lock implies **blocking** if the lock is not available (i.e. set by another thread)
  - threads waits until lock becomes available
API Locking Functions:
Testing Locks

- Test a lock and set it if it is unlocked (non-blocking)
- Fortran:
  
  ```fortran
  LOGICAL locked
  locked = OMP_TEST_LOCK(lockvar)
  ```

- C/C++:
  
  ```c
  int locked;
  locked = omp_test_lock(&lockvar);
  ```

- If the lock is already locked, returns with .FALSE. or zero, else sets it and returns .TRUE. or nonzero

- Only way to overlap work and resource sharing

API Locking Functions:
Example

```fortran
program uselock
integer omp_get_thread_num
logical omp_test_lock
external omp_get_thread_num, omp_test_lock
integer LCK, id
call OMP_INIT_LOCK(LCK)
!$OMP PARALLEL SHARED(LCK) PRIVATE(id)
  id=OMP_GET_THREAD_NUM()
  do while(.not. OMP_TEST_LOCK(LCK))
    call dosomework(id)
  end do
  print*, 'thread id=', id, 'calls work'
  call work(id)
  call OMP_UNSET_LOCK(LCK)
!$OMP END PARALLEL
call OMP_DESTROY_LOCK
end
```

Work while waiting for lock

protected by LCK
OpenMP library routines

- **Querying routines**
  - how many threads are there?
  - who am I?
  - where am I?
  - what resources are available?

- **Controlling parallel execution**
  - set number of threads
  - set execution mode
  - implement own synchronization constructs

---

OpenMP library routines (1)

Function calls return type **INTEGER** unless specified

- **OMP_GET_NUM_THREADS()**
  - yields number of threads in present environment
  - always 1 within sequentially executed region

  ```
  call OMP_SET_NUM_THREADS(nthreads)  \quad \text{(Subroutine call)}
  ```
  - set number of threads to a definite value
  - \( 0 \leq \text{nthreads} < \text{omp_get_max_threads()} \)
  - useful for specific algorithms
  - dynamic thread number assignment must be deactivated
  - overrides setting of `OMP_NUM_THREADS`

- **OMP_GET_THREAD_NUM()**
  - yields index of executing thread (0, \ldots, nthreads-1)

- **OMP_GET_NUM_PROCS()**
  - yields number of processors available for multithreading
  - `Always 8 for SR8000, # of processors for SGI (28 at RRZE)`

---
OpenMP library routines (2)

**OMP_GET_MAX_THREADS()**
maximum number of threads potentially available
(e.g., as set by operating environment/batch system)

**OMP_IN_PARALLEL()** (logical)
query whether program is executed in parallel or sequentially

In the example program, thread ID is used to distribute work.

OpenMP Constructs reviewed

- Control Constructs
  - Parallel Region
  - If
  - Work Sharing
    - Do
    - Schedule
    - Ordered
    - Sections
    - Single
- Data Constructs
  - ThreadPrivate
  - Data Scope
    - Shared
    - Private
    - FirstPrivate
    - LastPrivate
    - Reduction
    - CopyIn
    - Default
- Synchronization Constructs
  - OpenMP
  - Environment Functions
  - Lock Functions
  - Master
  - Critical
  - Barrier
  - Atomic
  - Ordered
- Environment Variables
- Runtime Library
  - OMP_SCHEDULE
    - Static
    - Dynamic
    - Dynamic_chunk
    - Guided
    - Guided_chunk
  - OMP_NUM_THREADS
  - OMP_DYNAMIC
  - OMP_NESTED
OpenMP Pitfalls:
Correctness

Three Types of Shared-Memory Errors

- **Race Condition**
  - Def.: Two threads access the same shared variable and at least one thread modifies the variable and the sequence of the accesses is undefined, i.e. unsynchronized
  - The result of a program depends on the detailed timing of the threads in the team.
  - This is often caused by unintended sharing of data

- **Deadlock**
  - Threads lock up waiting on a locked resource that will never become free.
    - Avoid lock functions if possible
    - At least avoid nesting different locks

- **Livelock**
  - multiple threads work forever on individual tasks
Example for race condition (1)

- The result varies unpredictably based on specific order of execution for each section.
- Wrong answers produced without warning!
- Solution: Apply synchronization constructs

```
A = B + C
B = A + C
C = B + A
```

```
!$omp parallel sections
  ic = 0
  !$omp parallel sections
  !$omp section
    a = b + c
    ic = 1
  !$omp section
    do while (ic < 1)
      !$omp flush(ic)
      end do
      b = a + c
      ic = 2
      ... (etc)
  !$omp end parallel sections
```

might effectively serialize code!

Example for race condition (2)

- The result varies unpredictably because the value of X isn't dependable until the barrier at the end of the do loop.
- Solution: Be careful when using NOWAIT

```
!$OMP PARALLEL SHARED (X), PRIVATE(TMP)
  ID = OMP_GET_THREAD_NUM()
!$OMP DO REDUCTION(+:X)
  DO 100 I=1,100
    TMP = WORK1(I)
    X = X + TMP
  100 CONTINUE
!$OMP END DO NOWAIT
  Y(ID) = WORK2(X,ID)
!$OMP END PARALLEL
```
OpenMP Pitfalls: Performance

- Thread startup and synchronization overhead
  - Every parallel and worksharing region takes time for the threads to start
    - Do not parallelize short loops! (cf. if clause)
  - Locks, critical regions, barriers synchronize threads
    - If possible, privatize data and synchronize only at the end
- False sharing
  - Avoid threads accessing data items close by in memory
  - False sharing can often be circumvented by padding
    - False sharing is disastrous, but can be fixed easily
- ccNUMA locality problems
  - Memory pages are not where access for threads is most efficient
  - Non-locality and congestion
  - Fixed by first-touch initialization
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?**

![Diagram showing memory locality problems and ccNUMA concept]

**“Golden Rule” of ccNUMA:**

A memory page gets mapped into the local memory of the processor that first touches it!

- Except if there is not enough local memory available
- This might be a problem, see later

**Caveat:** "touch" means "write", not "allocate"

**Example:**

```c
double *huge = (double*)malloc(N*sizeof(double));
// Memory not mapped yet
for(i=0; i<N; i++) // or i+=PAGE_SIZE
    huge[i] = 0.0; // Mapping takes place here!
```

- It is sufficient to touch a single item to map the entire OS page
Memory locality effects on ccNUMA

- **OpenMP triad on 2-socket dual-core Opteron**

![Graph showing memory locality effects](image)

- In-cache perf. largely untouched
- >2GB memory usage
- Switch to NT store (no RFO)

Memory Locality Problems

- **Locality of reference** is key to scalable performance on ccNUMA
  - Less of a problem with distributed memory (MPI) programming, but see below
- **What factors can destroy locality?**
  - **MPI programming** (see later):
    - processes lose their association with the CPU the mapping took place on originally
    - OS kernel tries to maintain strong affinity, but sometimes fails
  - **Shared Memory Programming** (OpenMP, ...):
    - threads losing association with the CPU the mapping took place on originally
    - improper initialization of distributed data
- **All cases:**
  - Other agents (e.g., OS kernel) may fill memory with data that prevents optimal placement of user data
Coding for Data Locality

- Simplest case: explicit initialization

```fortran
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
```

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

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

READ(1000) A

!$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) → see exercises

- **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

Coding for Data Locality:
Placement of static arrays or arrays of objects

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

```c++
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:
Parallel first touch for arrays of objects

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

```cpp
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);
}
```

Placement new!

Coding for Data Locality:
NUMA allocator for parallel first touch in STL vector

```cpp
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:
```cpp```
```cpp
vector<double,NUMA_Allocator<double> > x(1000000)
```
```cpp
```
ccNUMA problems beyond OpenMP

- Can locality problems appear even with correct initialization?
- Or even without using OpenMP?

- OS uses part of main memory for disk buffer (FS) cache
  - If FS cache fills part of memory, apps will probably allocate from foreign domains
  - \( \rightarrow \) non-local access!

- Remedies
  - Drop FS cache pages after user job has run (admin’s job)
  - User can run “sweeper” code that allocates and touches all physical memory before starting the real application

---

ccNUMA problems beyond OpenMP

- Real-world example: ccNUMA vs. UMA and the Linux buffer cache
- Compare two 4-way systems: AMD Opteron ccNUMA vs. Intel UMA, 4 GB main memory
- Run 4 concurrent triads after writing a large file
- Report performance vs. file size
- Drop FS cache after each data point