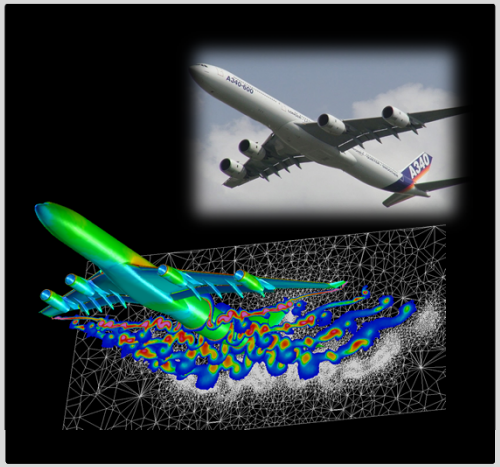

High Performance Computing

ADVANCED SCIENTIFIC COMPUTING

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LECTURE 6

Parallel Programming with OpenMP

September 26th, 2017
Room TG-227

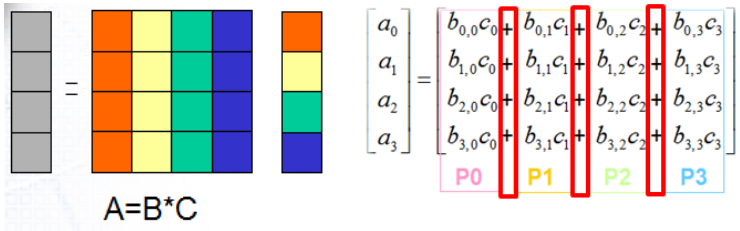
UNIVERSITY OF ICELAND
SCHOOL OF ENGINEERING AND NATURAL SCIENCES
FACULTY OF INDUSTRIAL ENGINEERING, MECHANICAL ENGINEERING AND COMPUTER SCIENCE

JÜLICH
FORSCHUNGSZENTRUM

Review of Lecture 5 – Parallel Algorithms & Data Structures

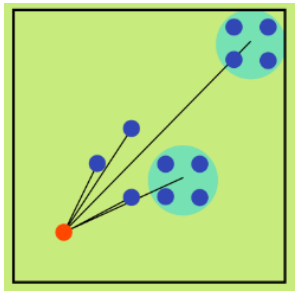
- Using MPI Collectives

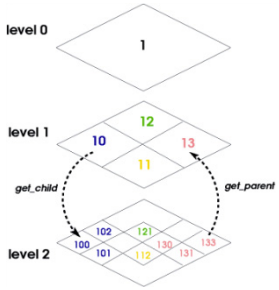

```
MPI_Scatter(x,CHUNK,MPI_DOUBLE,xpart,CHUNK,MPI_DOUBLE,0,MPI_COMM_WORLD);
MPI_Scatter(y,CHUNK,MPI_DOUBLE,ypart,CHUNK,MPI_DOUBLE,0,MPI_COMM_WORLD);

for (i=0; i<CHUNK; i++)
  zpart[i] = xpart[i] + ypart[i];

/* Collect the result */
MPI_Gather(zpart,CHUNK,MPI_DOUBLE,z,CHUNK,MPI_DOUBLE,0,MPI_COMM_WORLD);
```




```
/* Scatter matrix B */
MPI_Scatter(B,NCOLS,MPI_FLOAT,Bpart,NCOLS,MPI_FLOAT,0,MPI_COMM_WORLD);

/* Scatter vector C */
MPI_Scatter(C,1,MPI_FLOAT,Cpart,1,MPI_FLOAT, 0,MPI_COMM_WORLD);

/* Do the vector-scalar multiplication */
for(j=0; j < NCOLS; j++)
  Apart[j] = Cpart[0] * Bpart[j];

/* Reduce to matrix A */
MPI_Reduce(Apart,A,NCOLS,MPI_FLOAT,MPI_SUM, 0,MPI_COMM_WORLD);
```

- Tree-Code Approaches





- MPI Derived Datatypes

```
MPI_Type_contiguous( 3, oldtype, newtype );
```

```
MPI_Type_vector( 5, 2, 3, oldtype, newtype );
```

```
array_of_blocklengths[] = {2,3,1,2,2,2} /* below BL */
array_of_displacements[] = {3,9,12,15,18} /* below DIS */

MPI_Type_indexed ( 6, array_of_blocklengths, array_of_displacements, oldtype, newtype);
```

[1] Parallel Algorithms *[2] PEPC Webpage*

Outline of the Course

1. High Performance Computing
2. Parallelization Fundamentals
3. Parallel Programming with MPI
4. Advanced MPI Techniques
5. Parallel Algorithms & Data Structures
6. Parallel Programming with OpenMP
7. Hybrid Programming & Patterns
8. Debugging & Profiling Techniques
9. Performance Optimization & Tools
10. Scalable HPC Infrastructures & GPUs
11. Scientific Visualization & Steering
12. Terrestrial Systems & Climate
13. Systems Biology & Bioinformatics
14. Molecular Systems & Libraries
15. Computational Fluid Dynamics
16. Finite Elements Method
17. Machine Learning & Data Mining
18. Epilogue

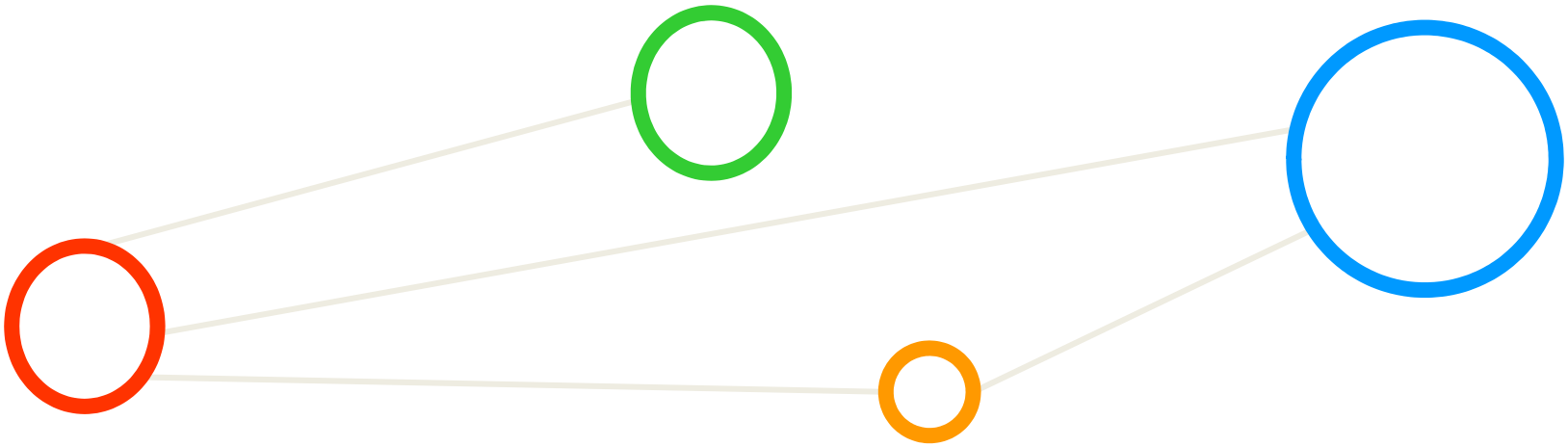
+ additional practical lectures for our hands-on exercises in context

Outline

- Shared-Memory Programming Concepts
  - Parallel and Serial Regions
  - Fork/Join & Master and Worker Threads
  - Standard & Portability
  - Hybrid Programming Motivation
  - Scientific Application Examples
- OpenMP Parallel Programming Basics
  - Basic building blocks
  - Local/shared variables & Loops
  - Synchronization & Critical Regions
  - Jacobi 2D Application Example
  - Selected Comparisons with MPI & Evolutions

- **Promises from previous lecture(s):**
- ***Lecture 1:* Lecture 6 will give in-depth details on the shared-memory programming model with OpenMP**
- ***Lecture 2:* Lecture 6 about OpenMP will include 'data parallelism on loops' methods that are useful here**
- ***Lecture 5:* Lecture 6 provides a detailed introduction to OpenMP used for shared memory programming**

Shared-Memory Programming Concepts



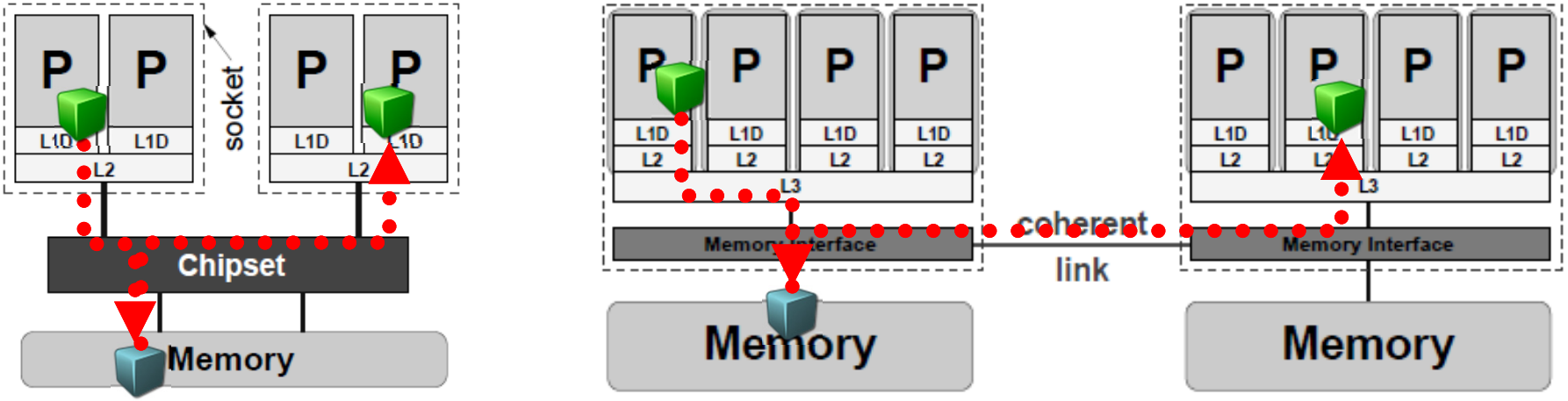
Shared-Memory Computers: Reviewed

- **A shared-memory parallel computer is a system in which a number of CPUs work on a common, shared physical address space**

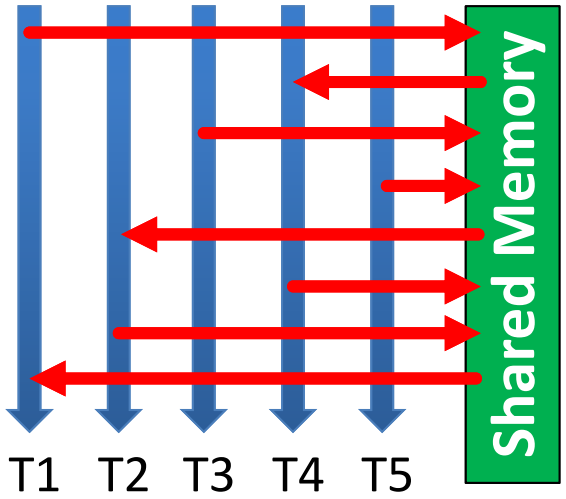
[3] Introduction to High Performance Computing for Scientists and Engineers

- Two varieties of shared-memory systems:
  1. Unified Memory Access (UMA)
  2. Cache-coherent Nonuniform Memory Access (ccNUMA)

(programming model: work on shared address space – 'local acess to memory')



Programming with Shared Memory using OpenMP



- **Shared-memory programming enables immediate access to all data from all processors without explicit communication**
- **OpenMP is dominant shared-memory programming standard today (v3)**

[4] OpenMP API Specification

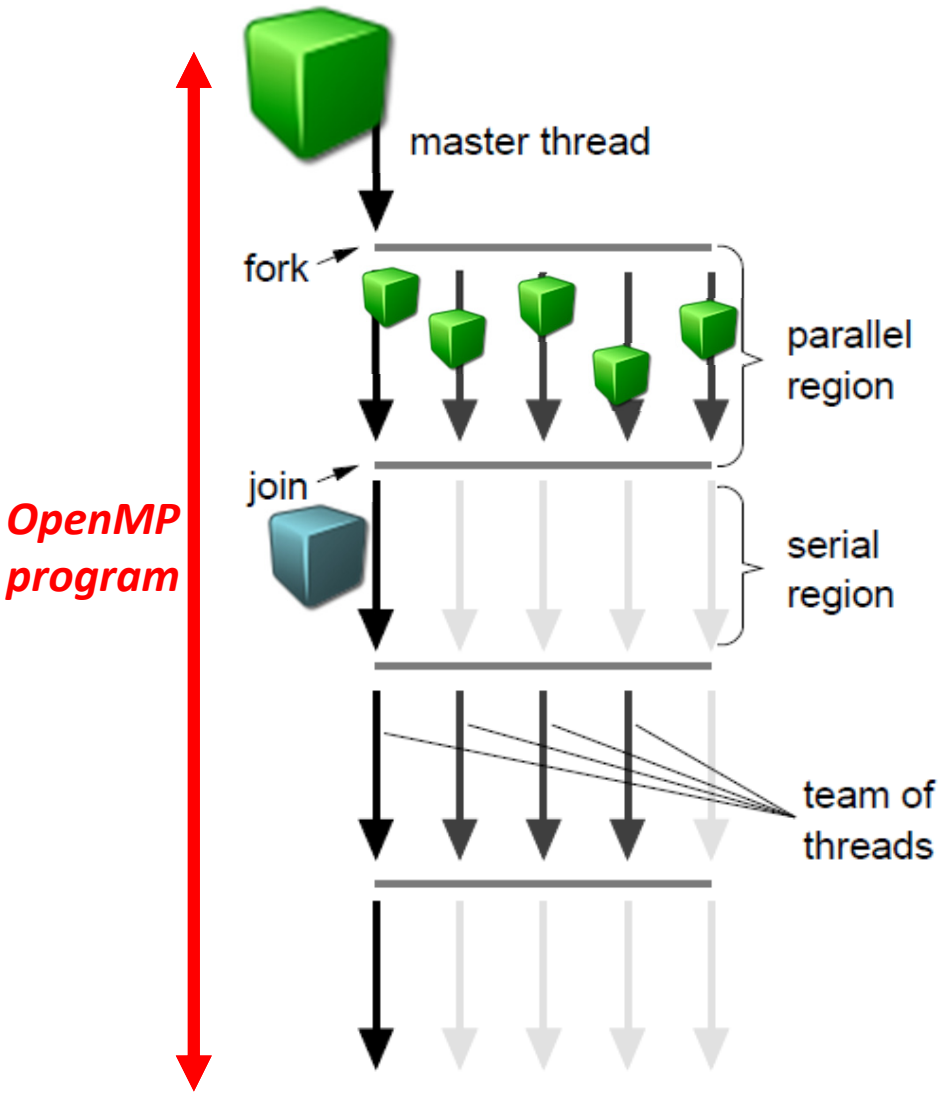
- OpenMP is a set of compiler directives to 'mark parallel regions'
- Bindings are defined for C, C++, and Fortran languages
- Threads TX are 'lightweight processes' that mutually access data
- (Shared-Memory concept itself is very old, like POSIX Threads)

What is OpenMP?

- OpenMP is a library for specifying 'parallel regions in serial code'
  - Defined by major computer hardware/software vendors → portability!
  - Enable scalability with parallelization constructs w/o fixed thread numbers
  - Offers a suitable data environment for easier parallel processing of data
  - Uses specific environment variables for clever decoupling of code/problem
  - Included in standard C compiler distributions (e.g. gcc)
- Threads are the central entity in OpenMP
  - Threads enable 'work-sharing' and share address space (where data resides)
  - Threads can be synchronized if needed
  - Lightweight process that share common address space with other threads
  - Initiating (aka 'spawning') n threads is less costly then n processes (e.g. variable space)

- **Recall 'computing nodes' are <u>independent</u> computing processors (that may also have N cores each) and that are all part of one big parallel computer**
- **Threads are lightweight processes that work with data in memory**

Parallel and Serial Regions

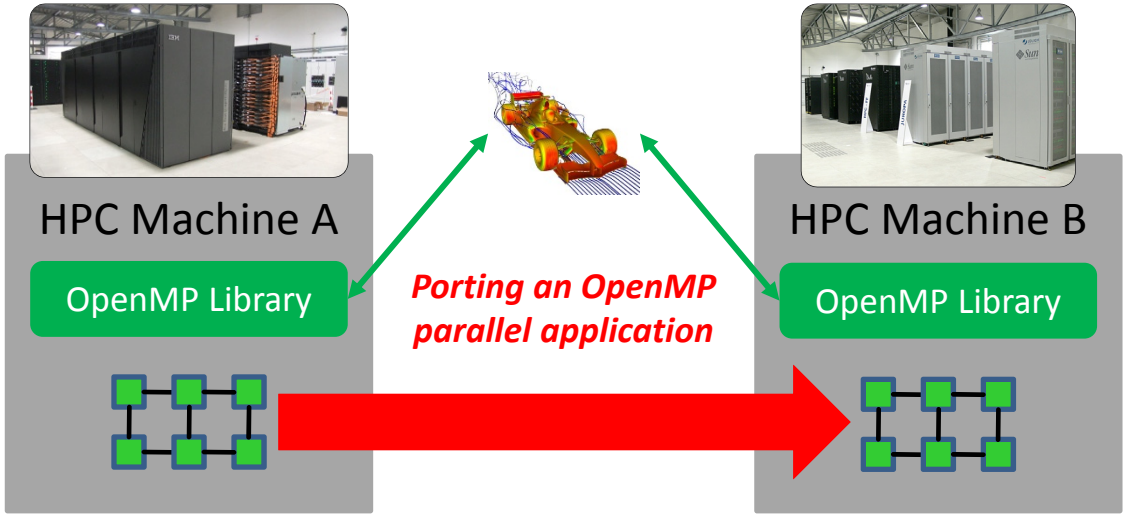


modified from [3] Introduction to High Performance Computing for Scientists and Engineers

- **fork() initiated by master thread (exists always) creates team of threads**
- **Team of threads concurrently work on shared-memory data <u>actively</u> in parallel regions**
- **join() initiates the 'shutdown' of the parallel region and terminates team of threads**
- **Team of threads maybe also put to sleep until next parallel region begins**
- **Number of threads can be different in each parallel region**

OpenMP Standard enables Portability

- Key reasons for requiring a standard programming library
  - Technical advancement in supercomputers is extremely fast
  - Parallel computing experts switch organizations and face another system
- Applications using proprietary libraries where not portable
  - Create whole applications from scratch or time-consuming code updates
- OpenMP is parallel programming model for UMA and ccNUMA

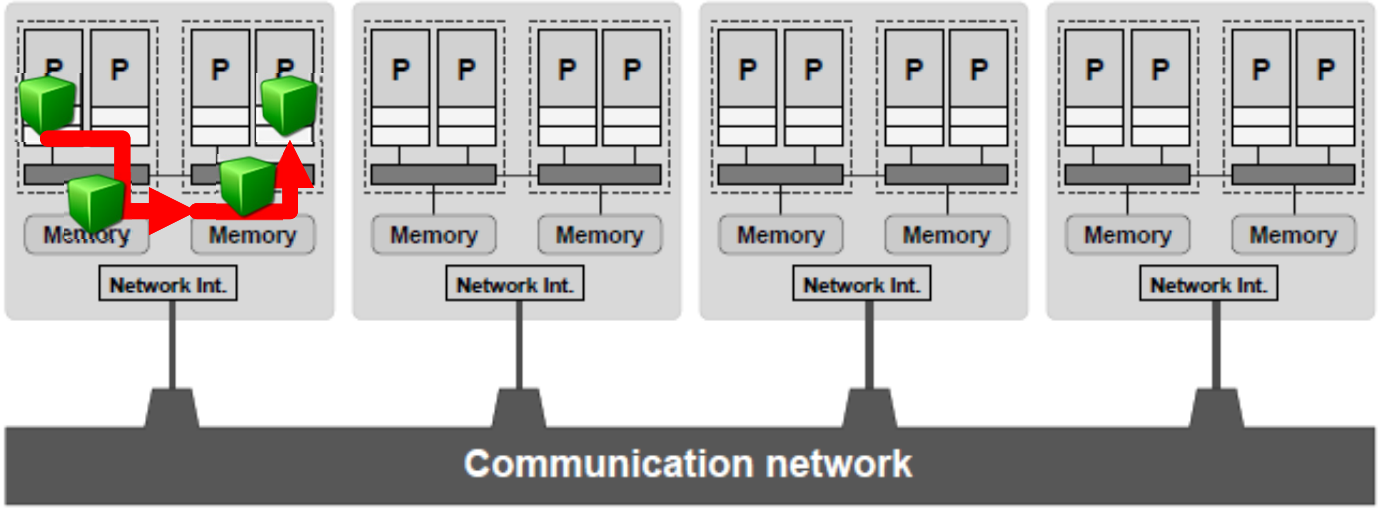


- **OpenMP is an open standard that significantly supports the portability of parallel shared-memory applications**
- **But different vendors might implement it differently**

Programming Hybrid Systems – Motivation

- Inefficient ‘on-node communications‘
  - MPI uses ‘buffering techniques‘ to transfer data (cf. Lecture 3 & 4)
  - Transfers may require ‘multiple memory copies‘ to get data from A to B
  - Comparable to a ‘memory copy‘ between different MPI processes

MPI ?



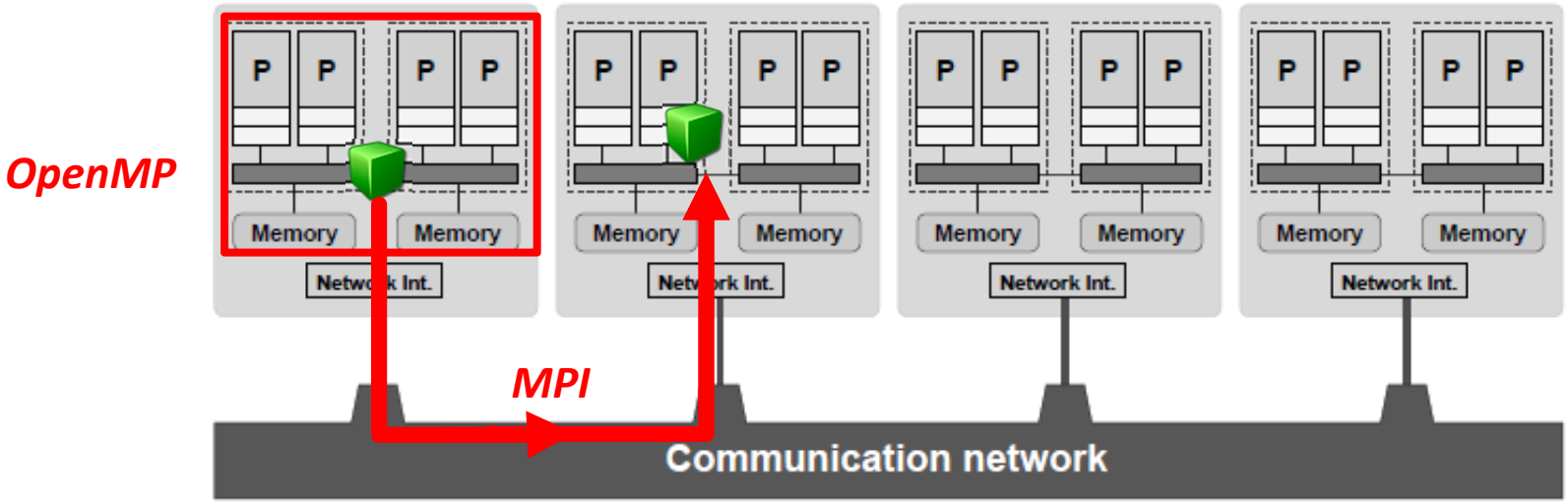
modified from [3] Introduction to High Performance Computing for Scientists and Engineers

- Take advantage of shared memory techniques where feasible
  - OpenMP threads can read memory on the same node

Hierarchical Hybrid Computers – Revisited

- **A hierarchical hybrid parallel computer is neither a purely shared-memory nor a purely distributed-memory type system but a mixture of both**
- **Large-scale 'hybrid' parallel computers have shared-memory building blocks interconnected with a fast network today**

[3] Introduction to High Performance Computing for Scientists and Engineers

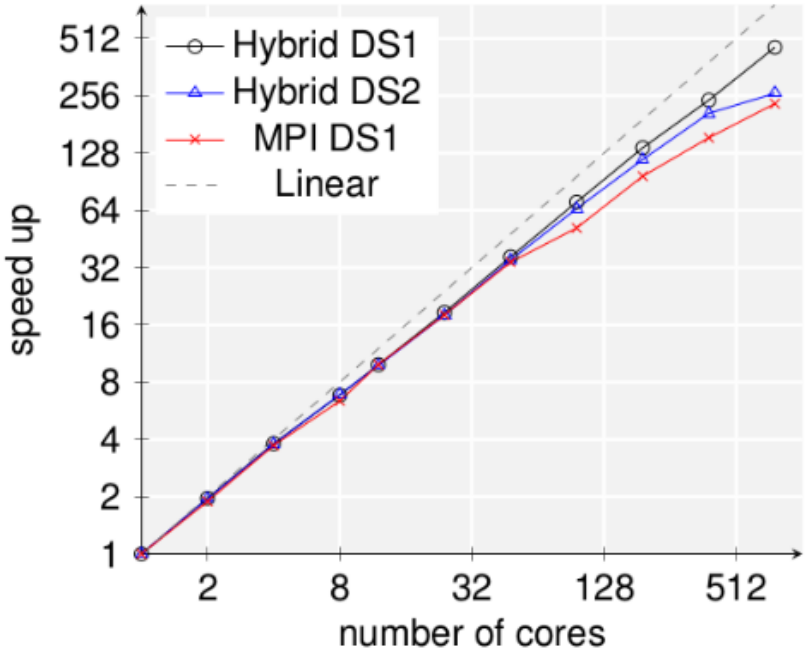


- Shared-memory nodes (i.e. ccNUMA) with local Network Int. (NI)
  - NI mediates connections to other remote 'SMP nodes'

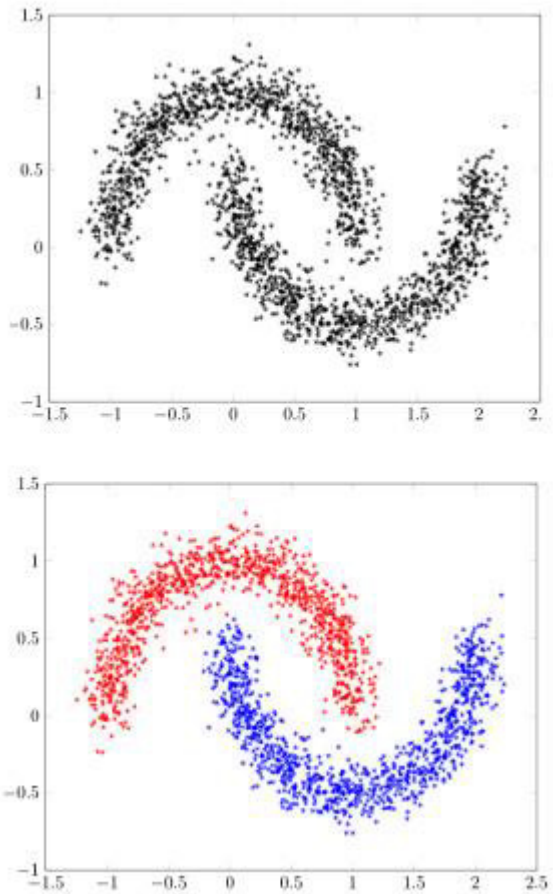
➢ **Lecture 7 offers more insights into hybrid programming jointly using both MPI and OpenMP**

Scientific Application Example: Data Mining & Clustering

- Hybrid data mining algorithm example
  - Parallel Density-based Spatial Clustering for Applications with Noise (DBSCAN)
  - Using MPI and OpenMP to scale better

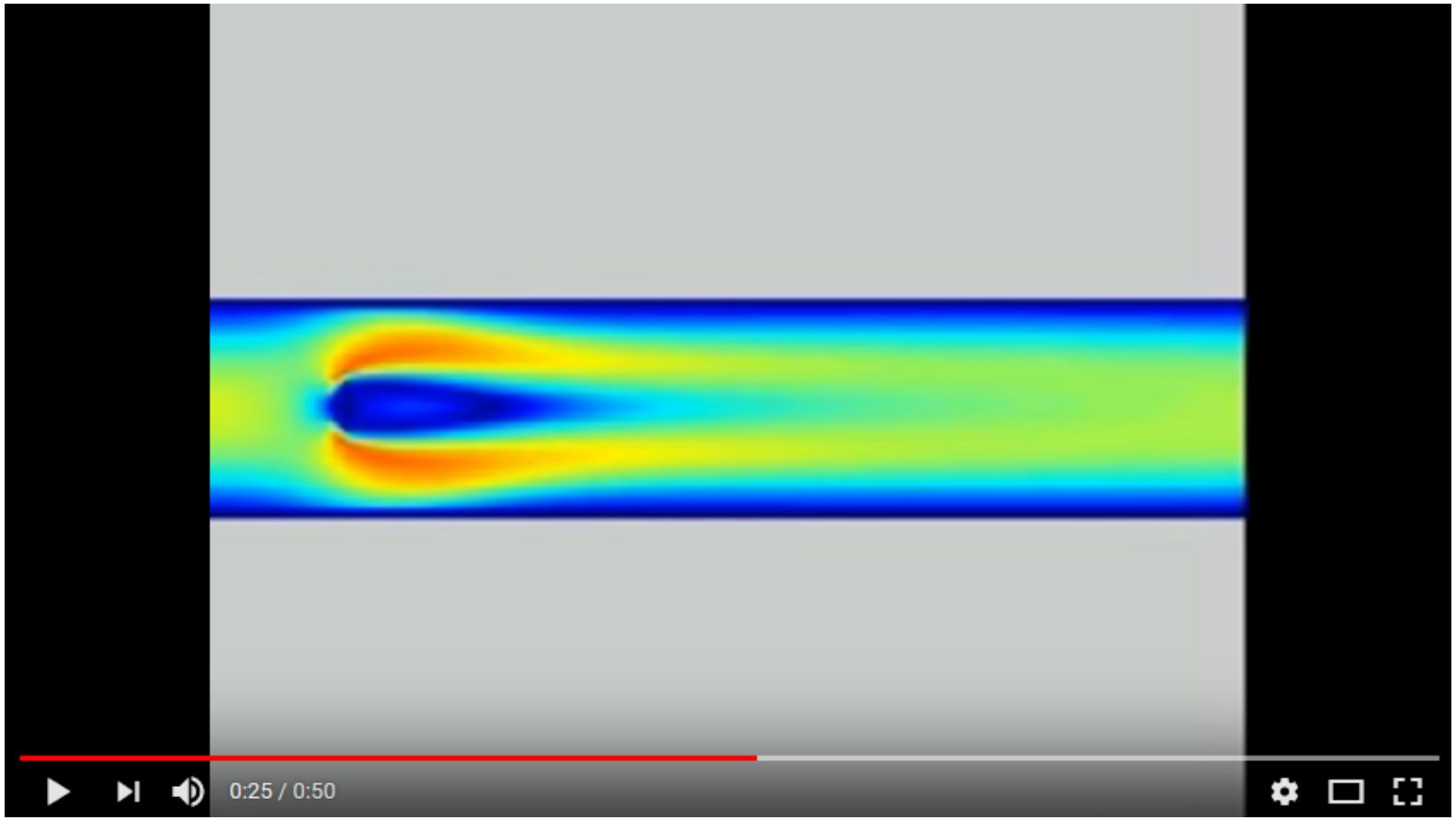


[5] M. Goetz & M. Riedel et al., 'Highly Parallel DBSCAN', MLHPC Workshop, SC2015



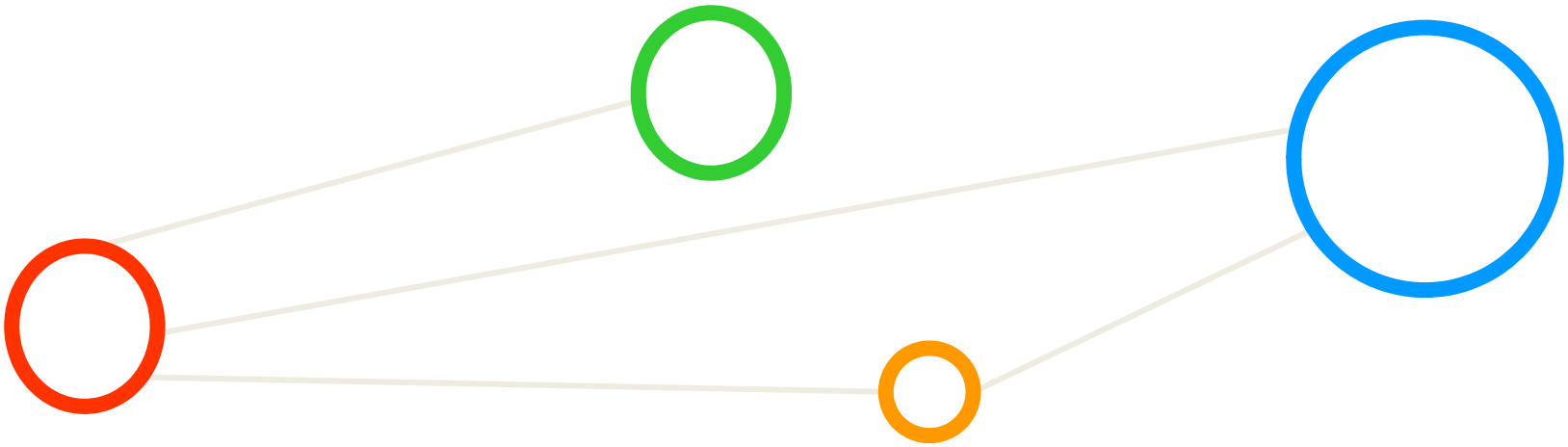
➢ **Lecture 17 gives insights into machine learning & data mining applications using OpenMP & MPI**

[Video] Scientific Application Example using OpenMP



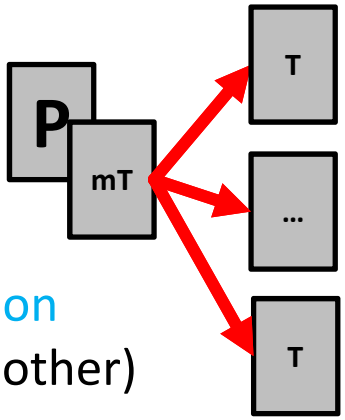
[6] Lattice Boltzmann – Flow past an obstacle, YouTube Video

OpenMP Parallel Programming Basics



Start 'Thinking' Parallel

- Parallel OpenMP programs know about the existence of a certain number of threads that all work togeter as part of a bigger picture
- OpenMP programs are written in a sequential programming language and some parts are executed in parallel
  - OpenMP programs run on a processor that 'spawns' numerous threads



- Parallelization of dedicated n parallel regions is key to the design in OpenMP (n = 1,2,3….)
  - E.g. loops/additions are good candidates for parallelization (if individual loop iterations are independent from each other)

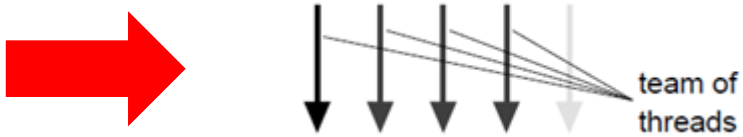
- Start with the basic building blocks using OpenMP
  - Defining code that enables 'parallel computing', step-by-step is possible

Number of Threads & Scalability

- **OpenMP programs should be always written in a way that it does not assume a specific number of threads → Scalable program**

- The real number of threads normally not known at compile time
  - (There are methods for doing it in the program → do not use them!)
  - Number is set in scripts and/or environment variable before executing

```
export OMP_NUM_THREADS=4
```

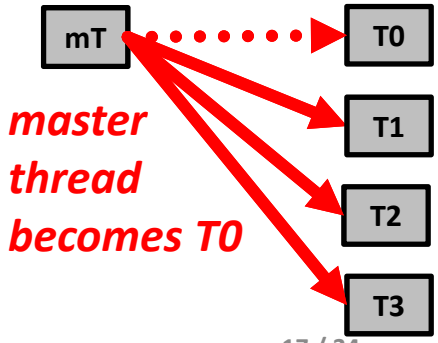


- Parallel programming is done without knowing number of threads

```
int main()
{
  #pragma omp parallel
  printf(„Hello World“);
}
```

compile & execute

```
./helloworld.exe
Hello World
Hello World
Hello World
Hello World
```



OpenMP Basic Building Blocks: Library & Sentinel

'standard fortran programming…'

```
  use omp_lib

  print *,'I am the
!$OMP PARALLEL
  call do_work_package(                                    )
!$OMP END PARALLEL
```

'standard C/C++ programming…'

```
  #include <omp.h>

  std::cout << "I am the master, and I am alone";
#pragma omp parallel
{
  do_work_package                                          );
}
```

- **The OpenMP library contains OpenMP API definitions**

- **The Sentinel is a special string that starts an OpenMP compiler directive**

- **Practice view: programming OpenMP in C/C++ and fortran is slightly different, but providing the same basic concepts (e.g. no end of parallel region in C/C++, local variables, etc.)**

OpenMP Basic Building Blocks: Unique Thread IDs

'standard fortran programming…'

```
  use omp_lib

  print *,'I am the
!$OMP PARALLEL
  call do_work_package(omp_get_thread_num(),omp_get_num_threads())
!$OMP END PARALLEL
```

'standard C/C++ programming…'

```
  #include <omp.h>

  std::cout << "I am the master, and I am alone";
#pragma omp parallel
{
  do_work_package(omp_get_thread_num(),omp_get_num_threads());
}
```

- **omp_get_thread_num() function provides unique Thread ID (0…n-1)**

- **omp_get_num_threads() function obtains number of <u>active</u> threads in the current parallel region**

- **do_work_package() routine code is now executed in parallel by each thread**
- **BUT also sub-routines of that routine are now executed in parallel**

OpenMP Basic Building Blocks: Private Variables (Fortran)

```
  integer :: bstart, bend, blen, numth, tid, i
  integer :: N
  double precision, dimension(N) :: a,b,c
  ...
!$OMP PARALLEL PRIVATE(bstart,bend,blen,numth,tid,i)
  numth = omp_get_num_threads()
  tid = omp_get_thread_num()
  blen = N/numth
  if(tid.lt.mod(N,numth)) then
    blen = blen + 1
    bstart = blen * tid + 1
  else
    bstart = blen * tid + mod(N,numth) + 1
  endif
  bend = bstart + blen - 1
  do i = bstart,bend
    a(i) = b(i) + c(i)
  enddo
!$OMP END PARALLEL
```

- **PRIVATE defines local variables for each thread**
- **Each thread <u>works independently</u> and thus needs space to 'store' local results**

- **Same code executed n times with n threads, BUT tid is unique and thus different for each thread**

- **Practice view: the real parallelization idea is here in the loop: the simple sum of two arrays**
- **For each value of i we can compute and store array values independently from each other**

Traditional HelloWorld Example (C/C++)

```
#include <omp.h>
#include <stdio.h>
int main(argc,argv)
int argc; char *argv[]; {

  int nthreads, tid;

  #pragma omp parallel private(tid)
  {
    tid = omp_get_thread_num();
    printf(„Hello World from thread = %d\n", tid);

    if (tid == 0)
    {
       nthreads = omp_get_num_threads();
       printf(„Number of threads in parallel region = %d\n", nthreads);
    }
  }
}
```

- Shared variable nthreads
- Local variable tid

- Simple Parallel Program
- Only the master (tid=0) provides output of how many threads are existing in the parallel region

➢ Practical lectures focus on MPI and not OpenMP, but both are important programming models

OpenMP Basic Building Blocks: Loops (do, for in C/C++)

```
  double precision :: pi,w,sum,x
  integer :: i,N=1000000

  pi = 0.d0
  w = 1.d0/N
  sum = 0.d0
!$OMP PARALLEL PRIVATE(x) FIRSTPRIVATE(sum)
!$OMP DO
  do i=1,n
    x = w*(i-0.5d0)
    sum = sum + 4.d0/(1.d0+x*x)
  enddo
!$OMP END DO
```

local sum exists, but where is the global sum?

```
!$OMP END PARALLEL
```

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

- **FIRSTPRIVATE() copies initial value of shared variable to local variable (simple init here otherwise problems in loop)**

- **DO loop (in front of usual do) distributes (automatically) loop iterations among threads as specifically supported 'work-sharing' construct)**

- **Smart programming support by OpenMP: Loops are very often part of scientific applications**
- **Less burden for programmer: no manual definition of local variables (e.g. i automatically localized)**

OpenMP Basic Building Blocks: Critical Regions

```
  double precision :: pi,w,sum,x
  integer :: i,N=1000000

  pi = 0.d0
  w = 1.d0/N
  sum = 0.d0
!$OMP PARALLEL PRIVATE(x) FIRSTPRIVATE(sum)
!$OMP DO
  do i=1,n
    x = w*(i-0.5d0)
    sum = sum + 4.d0/(1.d0+x*x)
  enddo
!$OMP END DO
!$OMP CRITICAL
  pi= pi + w*sum
!$OMP END CRITICAL
!$OMP END PARALLEL
```

- Local sum exists in each of the different threads
- We have n times the local variable value for sum now

- Race Condition in shared-memory: shared variable pi will be set concurrently by the different threads
- Value of pi depends on the exact order the threads access pi and assign wrong values

- Critical regions define a region within a parallel region where at most one thread at a time executes code (e.g. sum of new pi based on pi)

OpenMP Basic Building Blocks: Reduction

```
  double precision :: r,s
  double precision, dimension(N) :: a

  call RANDOM_SEED()
!$OMP PARALLEL DO PRIVATE(r) REDUCTION(+:s)
  do i=1,N
    call RANDOM_NUMBER(r)   ! thread safe
    a(i) = a(i) + func(r)   ! func() is thread safe
    s = s + a(i) * a(i)
  enddo
!$OMP END PARALLEL DO

  print *,'Sum = ',s
```

- Several operations are common in scientific applications
- +, *, -, &, |, ^, &&, ||, max, min

- REDUCTION() with operator + on variable s enables here …
- Starting with a local copy of s for each thread
- During progress of parallel region each local copy of s will be accumulated seperately by each thread
- At the end of the parallel region automatically synchronized and accumulated with resulting master thread variable

- Reduction operations are a smart alternative to manual critical regions defintions around operations of variables
- Reduction operation automatically localizes variable

Vector Addition in OpenMP – Revisited (cf. Lecture 5)

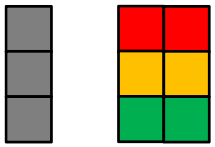
```
#include <omp.h>

int main(int argv, char **argv)
{
  int n, i;
  double *x, *y;

  /* Get input size */
  n = atoi(argv[1]);
  x = (double *)malloc(n*sizeof(double));
  y = (double *)malloc(n*sizeof(double));

  #pragma omp parallel for private(i) shared (x,y)
  for (i=0; i<n; i++)
  {
    x[i] = x[i] + y[i];
  }

  /* x containts the result for all vector elements */
}
```

'simplified demo code'

- The Sentinel is a special string that starts an OpenMP compiler directive
- Directive is optimized to enable a parallel loop (i.e. parallel for) starting a parallel region

- PRIVATE defines local variables for each thread
- Each thread <u>works independently</u> and thus needs space to 'store' local results – here i as index

- SHARED defines global variables that exist only one time
- Each thread <u>works independently</u> but SHARED variables can be written and read from all threads



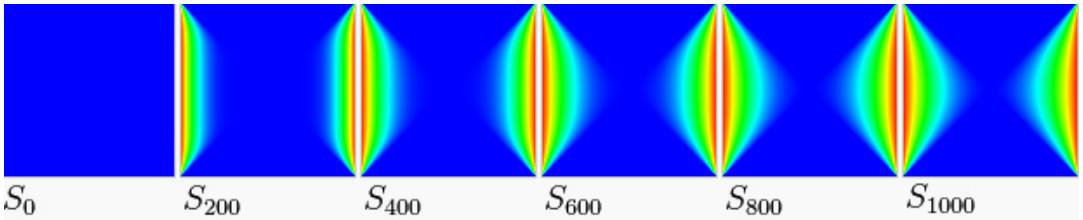
X = X+Y

Jacobi 2D Application Example – Revisited (cf. Lecture 2)

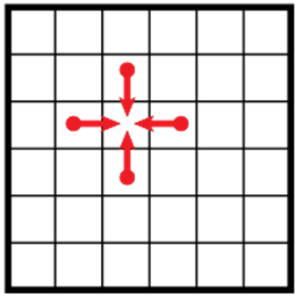
- **The Jacobi iterative method is a stencil-based iterative method used in numerical linear algebra**
- **Algorithm for determining the solutions of diagonally dominant system of linear equations**

- Solver
  - Each diagonal element is solved and approximate value is plugged in
  - The process is iterated until it converges
- Update function 2D Jacobi iterative method example
  - E.g. computes the arithmetic mean of a cell's four neighbours
  - E.g. solving diffusion equations (heat dissipation example)

[3] Introduction to High Performance Computing for Scientists and Engineers



[7] Wikipedia on 'stencil code'



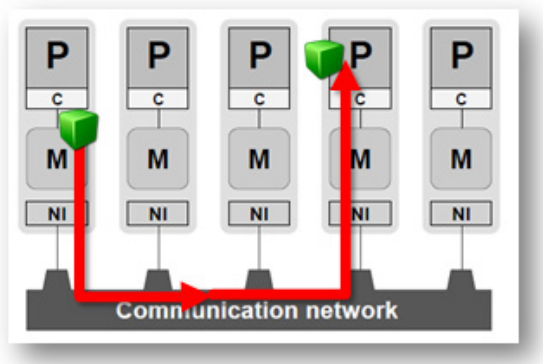
➢ **Lecture 7 will provide more details about stencil-based iterative methods and used patterns**

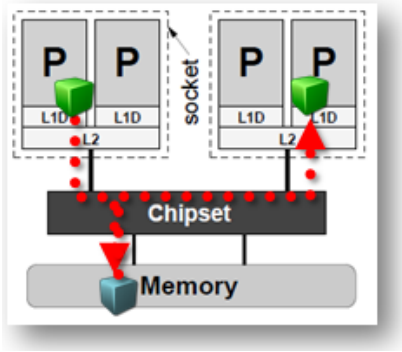
Advanced Example: 2D Jacobi Algorithm with OpenMP

```
double precision, dimension(0:N+1,0:N+1,0:1) :: phi
double precision :: maxdelta,eps
integer :: t0,t1
eps = 1.d-14        ! convergence threshold
t0 = 0 ; t1 = 1
maxdelta = 2.d0*eps
do while(maxdelta.gt.eps)
  maxdelta = 0.d0
!$OMP PARALLEL DO REDUCTION(max:maxdelta)
  do k = 1,N
    do i = 1,N
      ! four flops, one store, four loads
      phi(i,k,t1) = (  phi(i+1,k,t0) + phi(i-1,k,t0)
                     + phi(i,k+1,t0) + phi(i,k-1,t0) ) * 0.25
      maxdelta = max(maxdelta,abs(phi(i,k,t1)-phi(i,k,t0)))
    enddo
  enddo
!$OMP END PARALLEL DO
  ! swap arrays
  i = t0 ; t0=t1 ; t1=i
enddo
```

[3] Introduction to High Performance Computing for Scientists and Engineers

Selected Comparisons with MPI





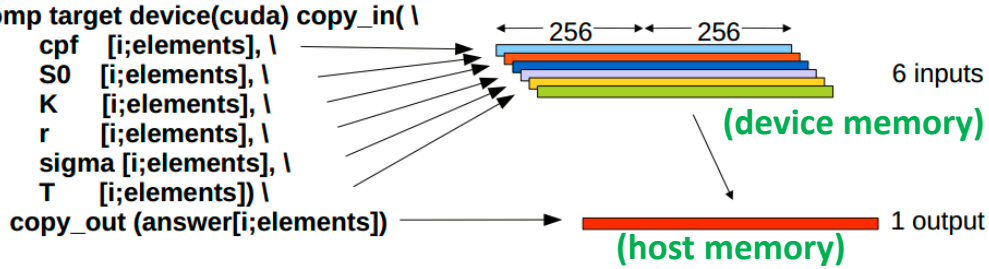
- Some aspects are similar, because both enable parallel computing
  - Obtaining unique IDs: MPI ranks vs. OpenMP thread-num
  - Master-worker approach (if rank==0 vs. if tid ==0)
- No explicit communication constructs to enable inter-process communication in OpenMP → assuming shared-memory
  - Data exchange: Message exchanges between processes vs. shared variable
  - Synchronization functions nevertheless exist in both: e.g. barriers
  - Clever automatisms for usual problems: MPI reduce vs. OpenMP reduction

DEEP-EST EU Project – OmpSs & OpenMP Evolutions

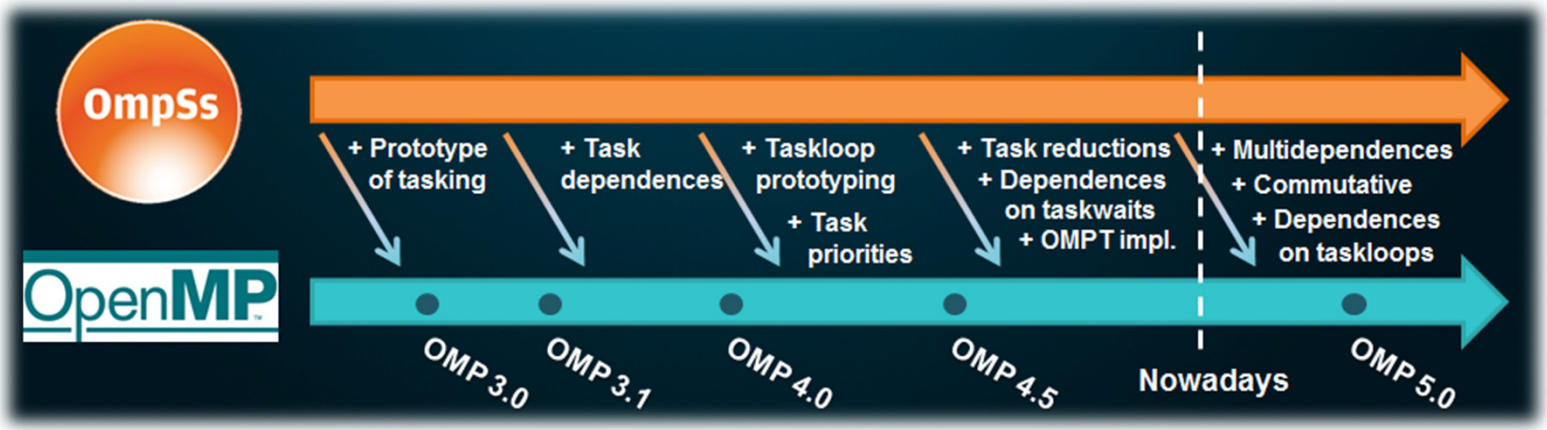
[9] DEEP-EST EU Project

[10] OmpSs Web page

```
#pragma omp target device(cuda) copy_in( \
        cpf    [i;elements], \
        S0     [i;elements], \
        K      [i;elements], \
        r      [i;elements], \
        sigma  [i;elements], \
        T      [i;elements]) \
copy_out (answer[i;elements])
```

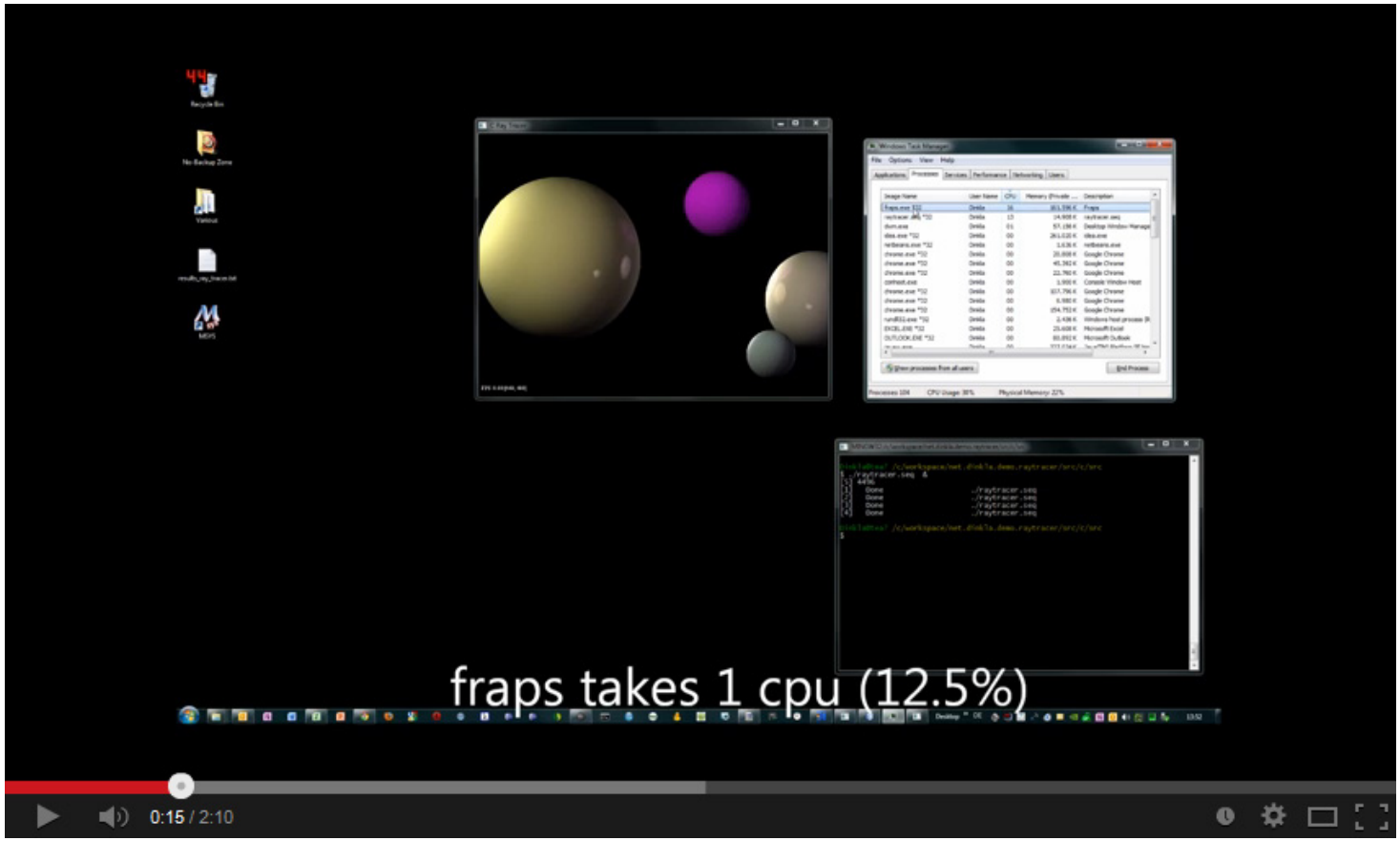


- OmpSs is an innovative programming model influencing OpenMP
  - Based on tasks and (data) dependencies – tasks as elementary unit of work
  - Extend OpenMP model: better data-flow & heterogenity (e.g. GPGPUs)



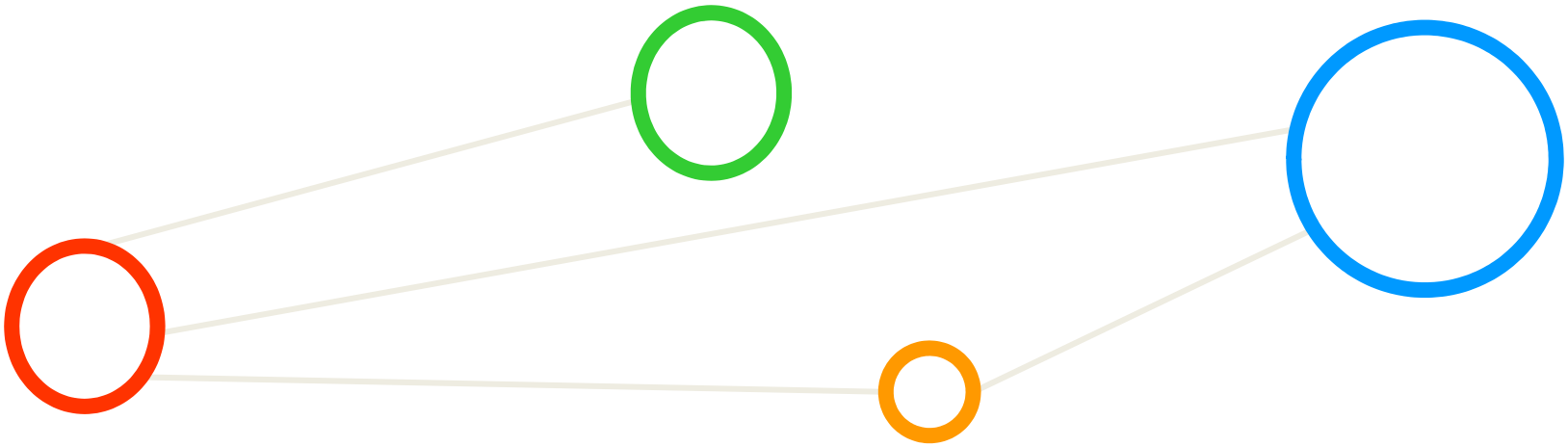
➢ **Lecture 10 will provide more details about the use of accelerators and the benefits of GPGPUs**

[Video] Raytracing Application with OpenMP



[8] Speeding up a Ray tracer with OpenMP, YouTube Video

Lecture Bibliography



Lecture Bibliography

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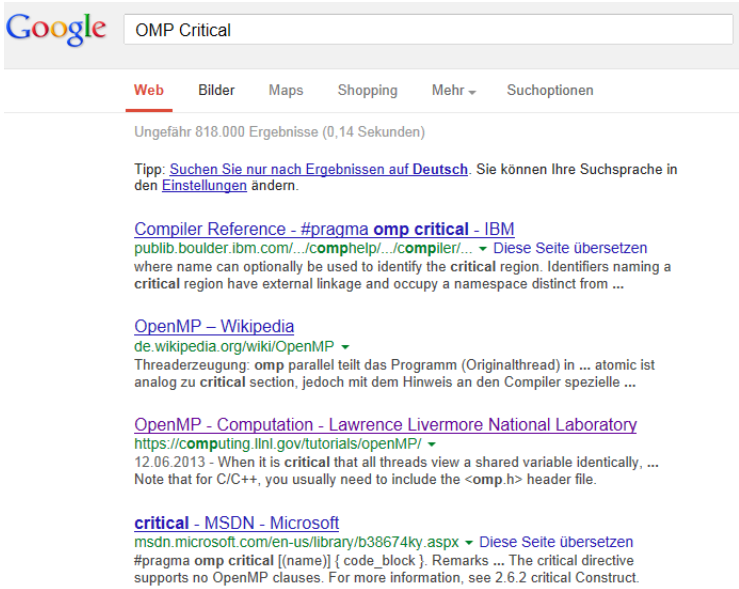
- [2] PEPC, FZ Juelich, Online: http://www.fz-juelich.de/ias/jsc/EN/AboutUs/Organisation/ComputationalScience/Simlabs/slpp/SoftwarePEPC/_node.html
- [3] Introduction to High Performance Computing for Scientists and Engineers, Georg Hager & Gerhard Wellein, Chapman & Hall/CRC Computational Science, ISBN 143981192X
- [4] The OpenMP API specification for parallel programming, Online: http://openmp.org/wp/openmp-specifications/
- [5] M. Goetz, C. Bodenstein, M. Riedel, '*HPDBSCAN – Highly Parallel DBSCAN',* Proceedings of the ACM/IEEE International Conference for High Performance Computing, Networking, Storage, and Analysis (SC2015), Machine Learning in HPC Environments (MLHPC) Workshop, USA, Online: https://dl.acm.org/citation.cfm?doid=2834892.2834894
- [6] Lattice Boltzmann – Flow past an obstacle, Online: https://www.youtube.com/watch?v=fspGcBpxguo
- [7] Wikipedia on 'stencil code', Online: http://en.wikipedia.org/wiki/Stencil_code
- [8] Speeding up a Ray tracer with OpenMP, YouTube Video, Online: http://www.youtube.com/watch?v=S9Z5MeQS_LU
- [9] DEEP-EST EU Project, Online: http://www.deep-projects.eu/
- [10] OmpSs Programming Model, Online: https://pm.bsc.es/ompss-docs/specs/01_introduction.html

Useful Collection on OpenMP Tutorials/Materials

- YouTube – ‘PRACE Video Tutorial – Introduction to OpenMP’, Online: http://www.youtube.com/watch?v=LyKA77PEM3o
- Introduction to OpenMP, HLRS Stuttgart, Online: https://fs.hlrs.de/projects/par/par_prog_ws/pdf/openmp-intro7.pdf
- Using OpenMP – Portable Shared Memory Parallel Programming, B. Chapman, G. Jost, R. Van der Pas (2008)
- Parallel Programming in OpenMP R. Chandra, L. Dagum, D. Kohr, D. Maydan, J. McDonald, R. Menon (2001)
- LLNL OpenMP Tutorial, Online: https://computing.llnl.gov/tutorials/openMP/

- **And if you don‘t find something:**
  ‚just google the OpenMP compiler directive or environment variable in question – good resources are out there‘:

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nodes
PB
community
Environment
different
Key
scientific
important
Science
centers
storage
basis
Infrastructure
files
model
international
SMAQ
etc
DKRZ
Use
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simulations
ENES
technologies
engineering
References
brain
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via
EUDAT
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IPCC
Big
Project
Data
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TB
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