Universität Zürich[UZH]

Hybrid parallel programming

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Open Source Macroeconomics Laboratory – BFI/UChicago

Including adapted teaching material from books, lectures and presentations by
B. Barney, B. Cumming, W. Gropp, G. Hager, M. Martinasso, R. Rabenseifner, O. Schenk, G. Wellein

Day 4, Thursday – Aug 3rd

1. Hybrid parallelism (8.00-9.00 – hands on).

2. Hybridize some of the projects together (9.15-10.00).

3. Advanced topics (10.15-11.00).

4. Start to present results from the projects (11.10 – 11.50).

5. Exercise sheet related to the day's topic
   (11.50-12.00 – hands on).

Outline

Hybrid parallelism in general

- Recap hardware & programming models

- Merging OpenMP & MPI

- “Hello World” in hybrid

Putting things together:

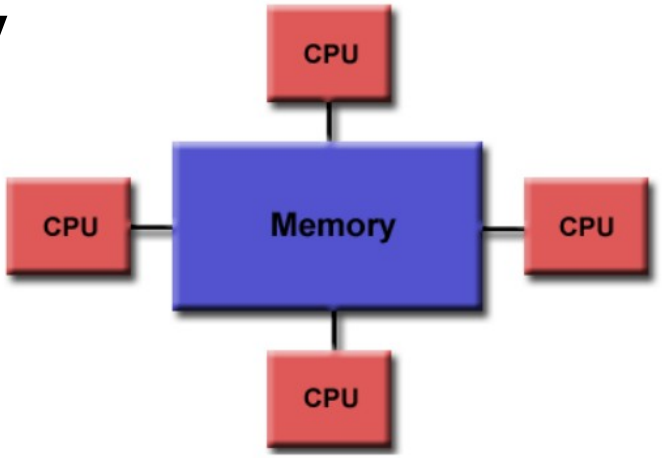
- Time Iteration, Adaptive Sparse Grids, HPC

Shared memory systems – OpenMP

- Process can access same GLOBAL memory

- Uniform Memory Access (UMA) model

- Access time to memory is uniform.
- Local cache, all other peripherals are shared.

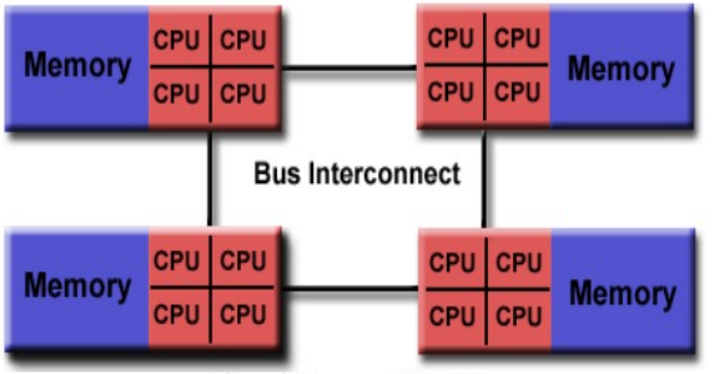


Shared Memory (UMA)

- Non-Uniform Memory Access (NUMA) model

- Memory is physically distributed among processors.
- Global virtual address spaces accessible from all processors.
- Access time to local and remote data is different.

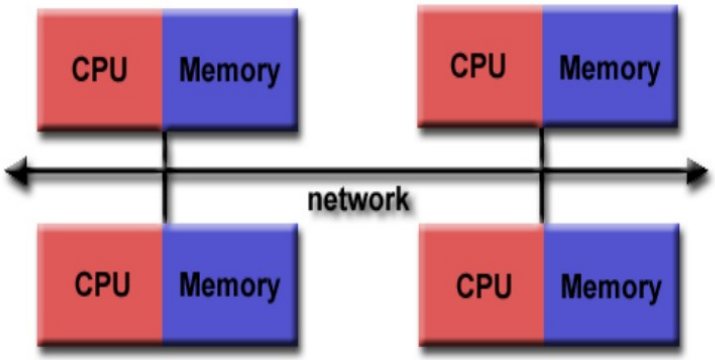
→ **OpenMP**, but other solutions available (e.g. Intel's TBB).



Shared Memory (NUMA)

Distributed-memory parallel programming – MPI

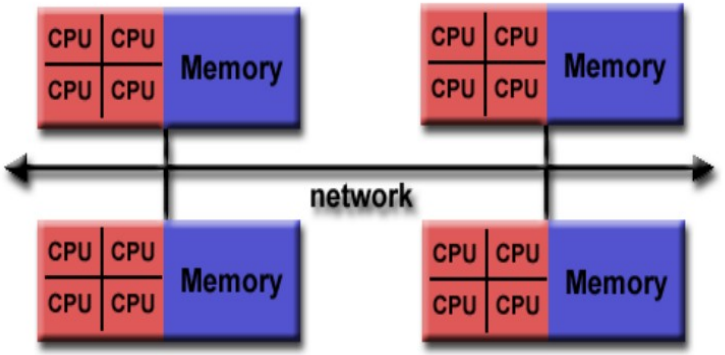
- We need to use explicit message passing,
  i.e., communication between processes:
  → Most tedious and complicated but also
  the most flexible parallelization method.



- Message passing is required if
  a parallel computer is of **distributed-memory**
  type, i.e., if there is no way for one processor
  to directly access the address space of another.

- However, it can also be regarded
  as a programming model and used
  on shared-memory or **hybrid systems** as well.

→ **Message Passing Interface (MPI)**.

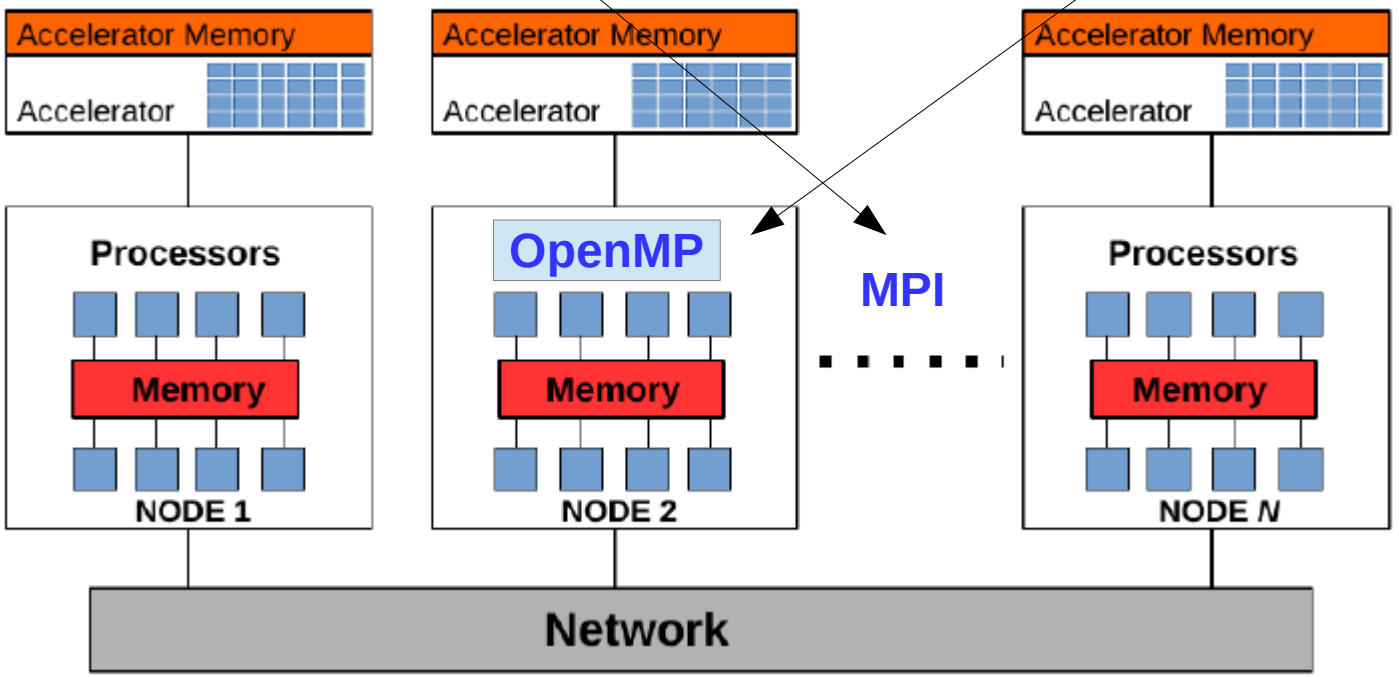


Today's HPC systems

- Efficient programming of clusters of **shared memory (SMP)** **nodes**

- Hierarchical system layout

- Hybrid programming seems natural:
  - → **MPI among the nodes.**
  - → **Shared memory programming inside of each SMP node – OpenMP.**



Hybrid parallelism with MPI and OpenMP

When Does Hybridization Make Sense?

- When one wants to scale a shared memory OpenMP application for use on **multiple SMP nodes** in a cluster.

- When one wants to reduce an MPI application's sensitivity to becoming communication bound.

- **When one is designing a parallel program (nowadays) from the very beginning.**

- for 8/16/32/64/...ranks per multi-core node, this can have scaling problems with many nodes/MPI ranks.

Hybridization Using MPI and OpenMP

- facilitates cooperative shared memory (OpenMP) programming across clustered SMP nodes.

- MPI facilitates **communication** among SMP nodes.

- OpenMP manages the **workload** on each SMP node.

- **MPI and OpenMP are used in tandem** to manage the overall concurrency of the application.

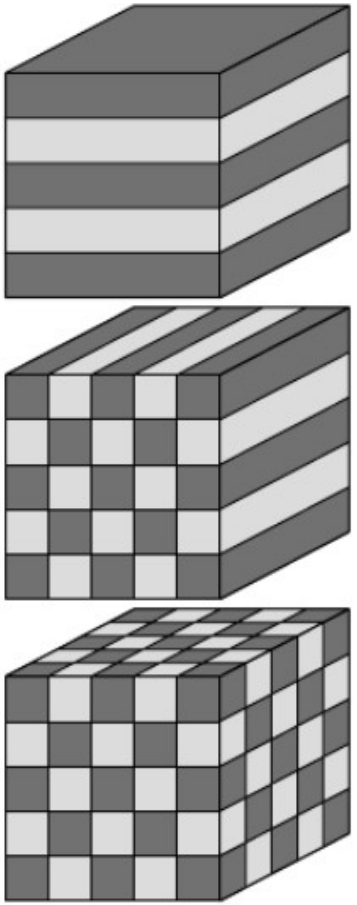
The hybrid MPI & OpenMP model

The MPI only model assigns **one process per core**:

- → for 8/16/32/64/...ranks per multi-core node, this can have scaling problems with many nodes/MPI ranks.
- → **the amount of data passed around in messages increases as number of ranks increases**.
- → to take advantage of shared cache and DRAM on a socket, why not use threads on the socket/node, and pass messages between sockets/nodes? (it's a lot faster then sending messages around)

The hybrid MPI & OpenMP model has light-weight threads that share on-node memory.

Domain decomposition



"Slabs"

$$c_{1d}(L,N) = L \cdot L \cdot w \cdot 2 = 2wL^2$$

"Poles"

$$c_{2d}(L,N) = L \cdot \frac{L}{\sqrt{N}} \cdot w \cdot (2+2) = 4wL^2N^{-1/2}$$

"Cubes"

$$c_{3d}(L,N) = \frac{L}{\sqrt[3]{N}} \cdot \frac{L}{\sqrt[3]{N}} \cdot w \cdot (2+2+2) = 6wL^2N^{-2/3}$$

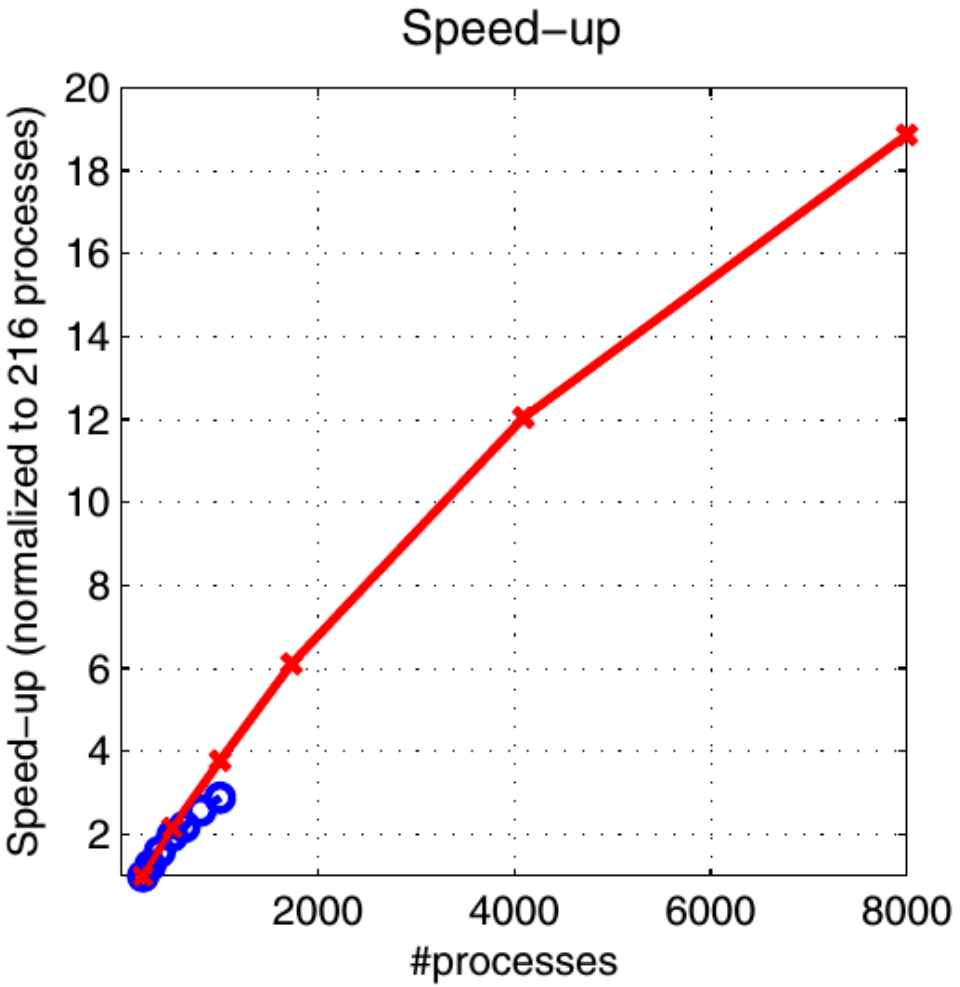
Figure 10.9: 3D domain decomposition of a cubic domain of size L^3 (strong scaling) and periodic boundary conditions: Per-process communication volume $c(L,N)$ for a single-site data volume w (in bytes) on N processes when cutting in one (top), two (middle), or all three (bottom) dimensions.

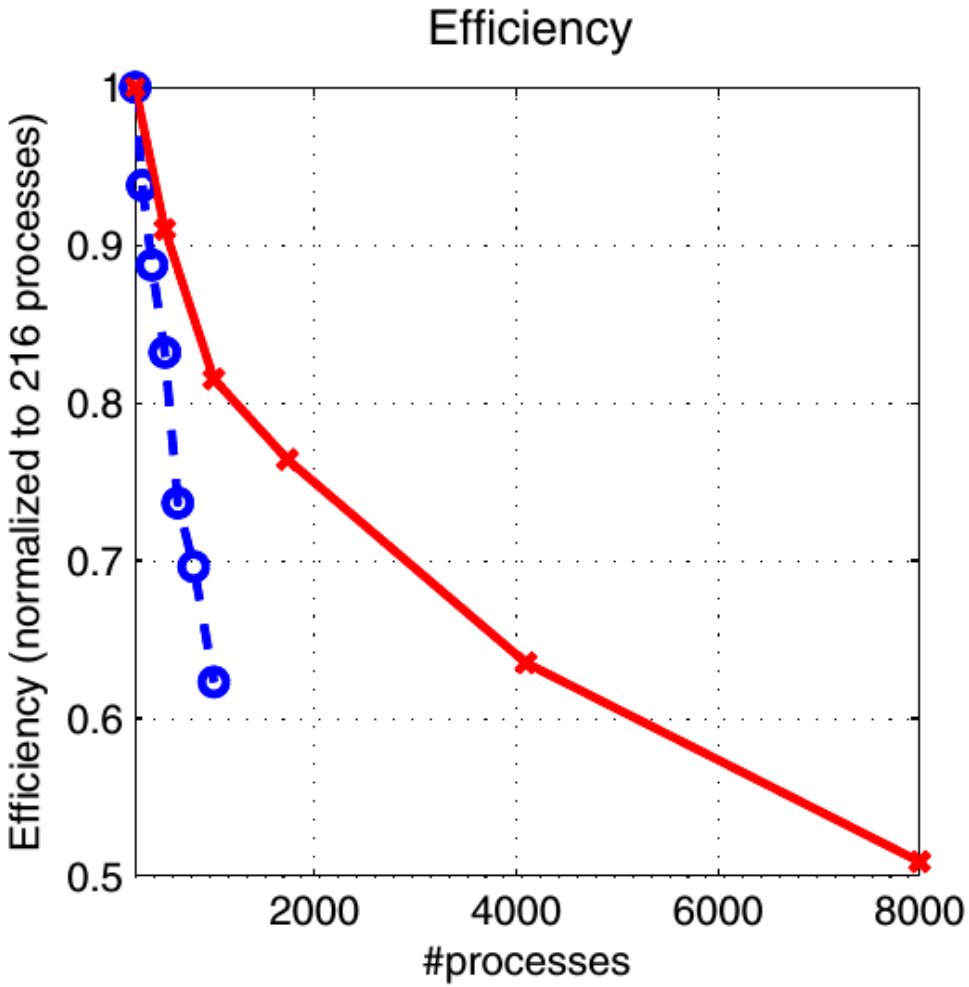
From Hager & Wellein (2011)

Example: Scaling “MPI” vs. “Hybrid”

See, e.g., Käppeli et al. (2011) http://iopscience.iop.org/article/10.1088/0067-0049/195/2/20/pdf

Hybrid parallelization:
→ Reduces the amount of memory consumption.
→ Reduces the amount of communication required.





Hybrid parallelism with MPI and OpenMP

Recall MPI

- Provides a familiar and explicit means to use message passing on distributed memory clusters.
- Has implementations on many architectures and topologies.
- Is the de-facto standard for distributed memory communications.
- Requires that program state synchronization must be handled explicitly due to the nature of distributed memory.
- data goes to the process.
- program correctness is an issue, but not big compared to those inherent to OpenMP.

OpenMP

- Allows for implicit intra-node communication, which is a shared memory paradigm.
- Provides for efficient utilization of shared memory SMP systems.
- Facilitates relatively easy threaded programming.
- Does not incur the overhead of message passing, since communication among threads is implicit.
- Is the de-facto standard, and is supported by most major compilers (Intel, IBM, gcc, etc).
- The process goes to the data program correctness is an issue since all threads can update shared memory locations.

The best from both worlds

- MPI allows for inter-node communication.

- MPI facilitates efficient inter-node reductions and sending of complex data structures.

- Program synchronization is explicit.

- A common execution scenario: a single MPI process is launched on each SMP node in the cluster.

- Each process spawns *N* threads on each SMP node.

- At some global sync point, the master thread on each SMP communicate with one another.

- The threads belonging to each process continue until another sync point or completion.

Memory consumption & mapping

- Memory consumption MPI & OpenMP with n threads per MPI process:
  → Duplicated data may be reduced by factor *n*.

- How many threads per MPI process?
  SMP node = with *m* sockets (NUMA domains) and *n* cores/socket

- How many threads (i.e., cores) per MPI process?
  → Too few threads, too much memory consumption

- Optimum:
  → somewhere between 1 and m x n threads per MPI process.

- Typical optima:
  → 1 MPI process per socket.
  → 2 MPI processes per socket.
  → Seldom: 1 MPI process per whole SMP node.

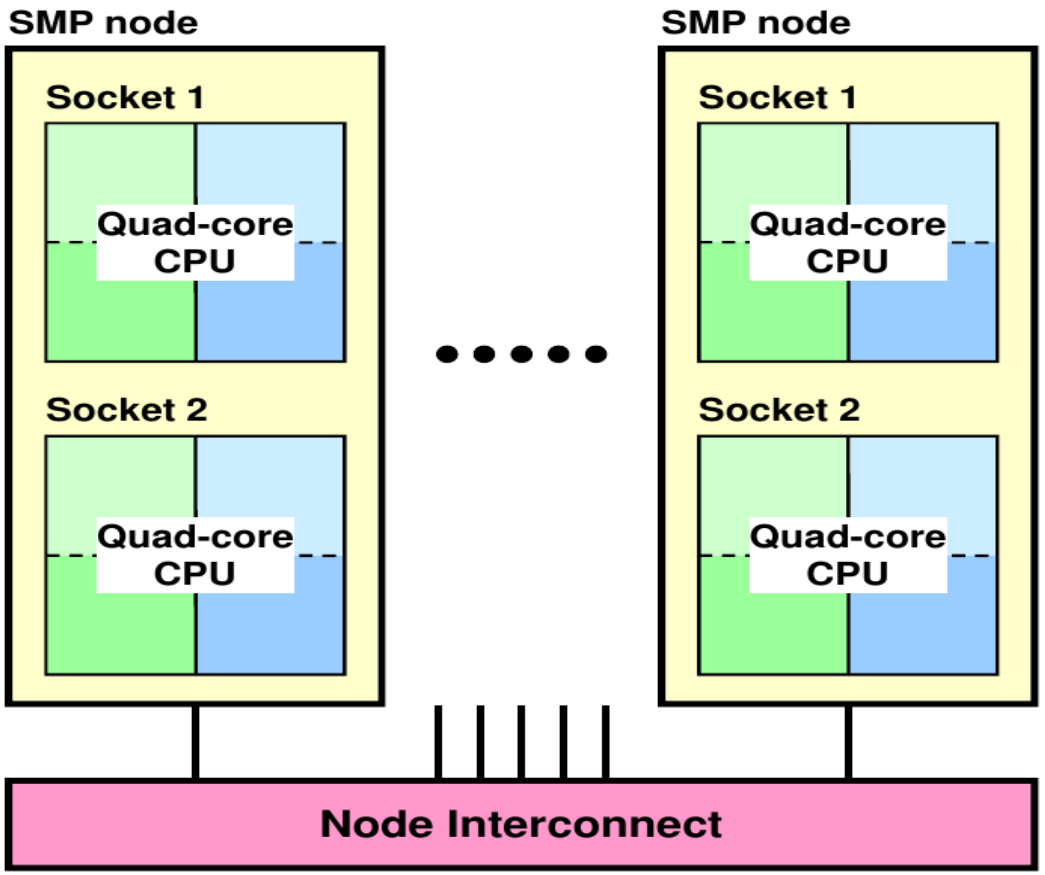
A node

- Which programming model is fastest?

- MPI everywhere?

- Fully hybrid MPI & OpenMP?

- Something between? (Mixed model)



Mapping (2)

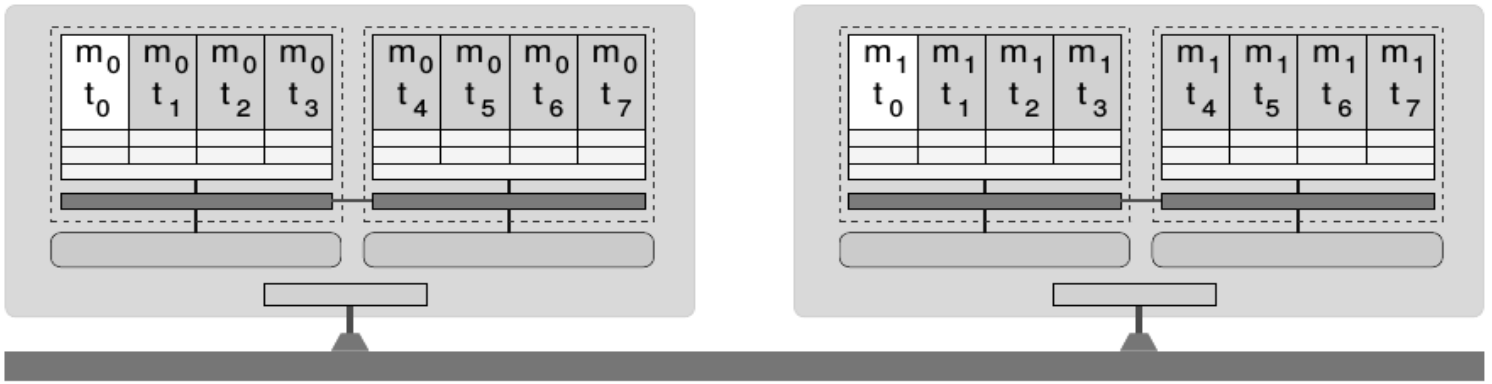


Figure 11.3: Mapping a single MPI process with eight threads to each node.

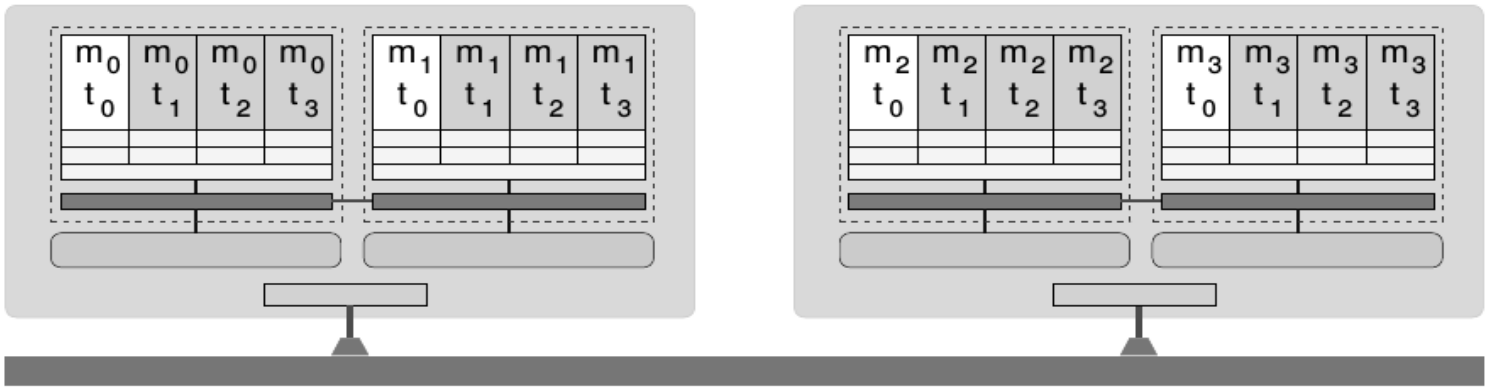


Figure 11.4: Mapping a single MPI process with four threads to each socket (L3 group or locality domain).

From Hager & Wellein (2011)

Mapping (3)

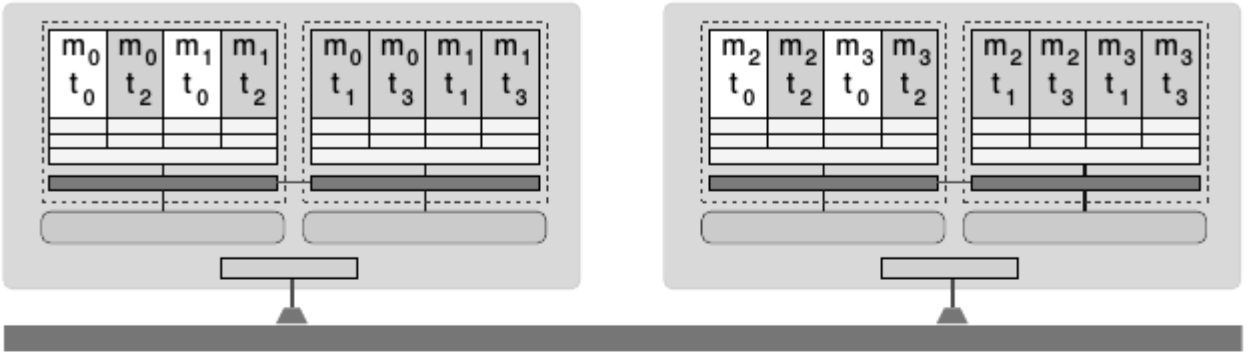


Figure 11.5: Mapping two MPI processes to each node and implementing a round-robin thread distribution.

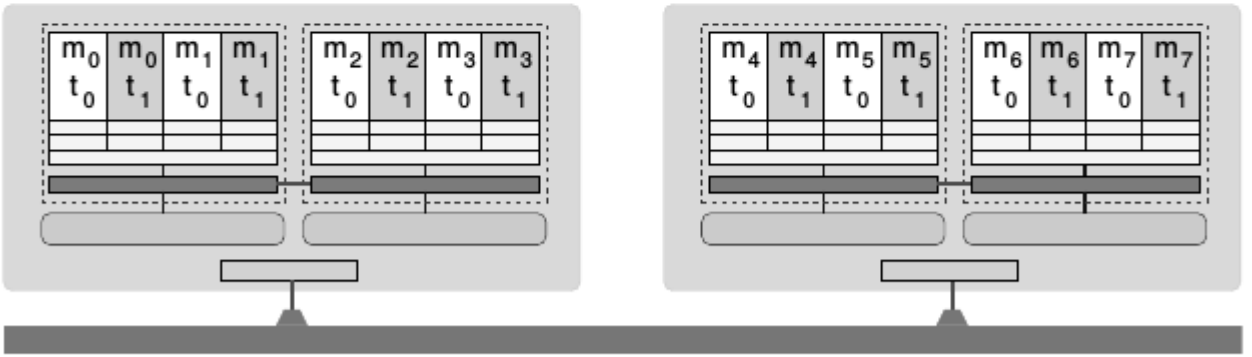


Figure 11.6: Mapping two MPI processes with two threads each to a single socket.

From Hager & Wellein (2011)

Opportunities

Algorithmic opportunities due to larger physical domains inside of each MPI process:

→ If MPI domain decomposition is based on physical zones:
Nested Parallelism Outer loop with MPI / inner loop with OpenMP.

→ Load-Balancing: Using OpenMP dynamic and guided work sharing

→ Memory consumption: Significantly reduction of replicated data on MPI level.

→ Reduced MPI scaling problems: Significantly reduced number of MPI processes

→ Opportunities, if MPI speed-up is limited due to algorithmic problem

→ Significantly reduced number of MPI processes.

Basic MPI/OpenMP programming models

- The basic idea of a hybrid OpenMP/MPI programming model is to allow any MPI process to spawn a team of OpenMP threads in the same way as the master thread does in a pure OpenMP program.

- Inserting OpenMP compiler directives into an existing MPI code is a straightforward way to build a first hybrid parallel program.

- Following the guidelines of good OpenMP programming, compute intensive loop constructs are the primary targets for OpenMP parallelization in a naive hybrid code.

- Before launching the MPI processes one has to specify the maximum number of OpenMP threads per MPI process in the same way as for a pure OpenMP program.

- At execution time each MPI process activates a team of threads (being the master thread itself) whenever it encounters an OpenMP parallel region.

- There is no automatic synchronization between the MPI processes for switching from pure MPI to hybrid execution, i.e., at a given time some MPI processes may run in completely different OpenMP parallel regions, while other processes are in a pure MPI part of the program.

- Synchronization between MPI processes is still restricted to the use of appropriate MPI calls.

A common way to implement hybrid paralleism

Fortran

```
include 'mpif.h'
program hybsimp


call MPI_Init(ierr)
call MPI_Comm_rank (...,irank,ierr)
call MPI_Comm_size (...,isize,ierr)
! Setup shared mem, comp. & Comm

!$OMP parallel do
   do i=1,n
     <work>
   enddo
!  compute & communicate

call MPI_Finalize(ierr)
end
```

C/C++

```
#include <mpi.h>
int main(int argc, char **argv){
 int rank, size, ierr, i;

 ierr= MPI_Init(&argc,&argv[]);
 ierr= MPI_Comm_rank (...,&rank);
 ierr= MPI_Comm_size (...,&size);
//Setup shared mem, compute & Comm

#pragma omp parallel for
   for(i=0; i<n; i++){
     <work>
   }
// compute & communicate

 ierr= MPI_Finalize();
```

Example:”hello world hybrid”

1. go to OSM_Lab/HPC_day4/code_day4/hybrid:

> cd OSM_Lab/HPC_day4/code_day4/hybrid

2. Have a look at the code

> vi 1a.hello_world_hybrid.cpp

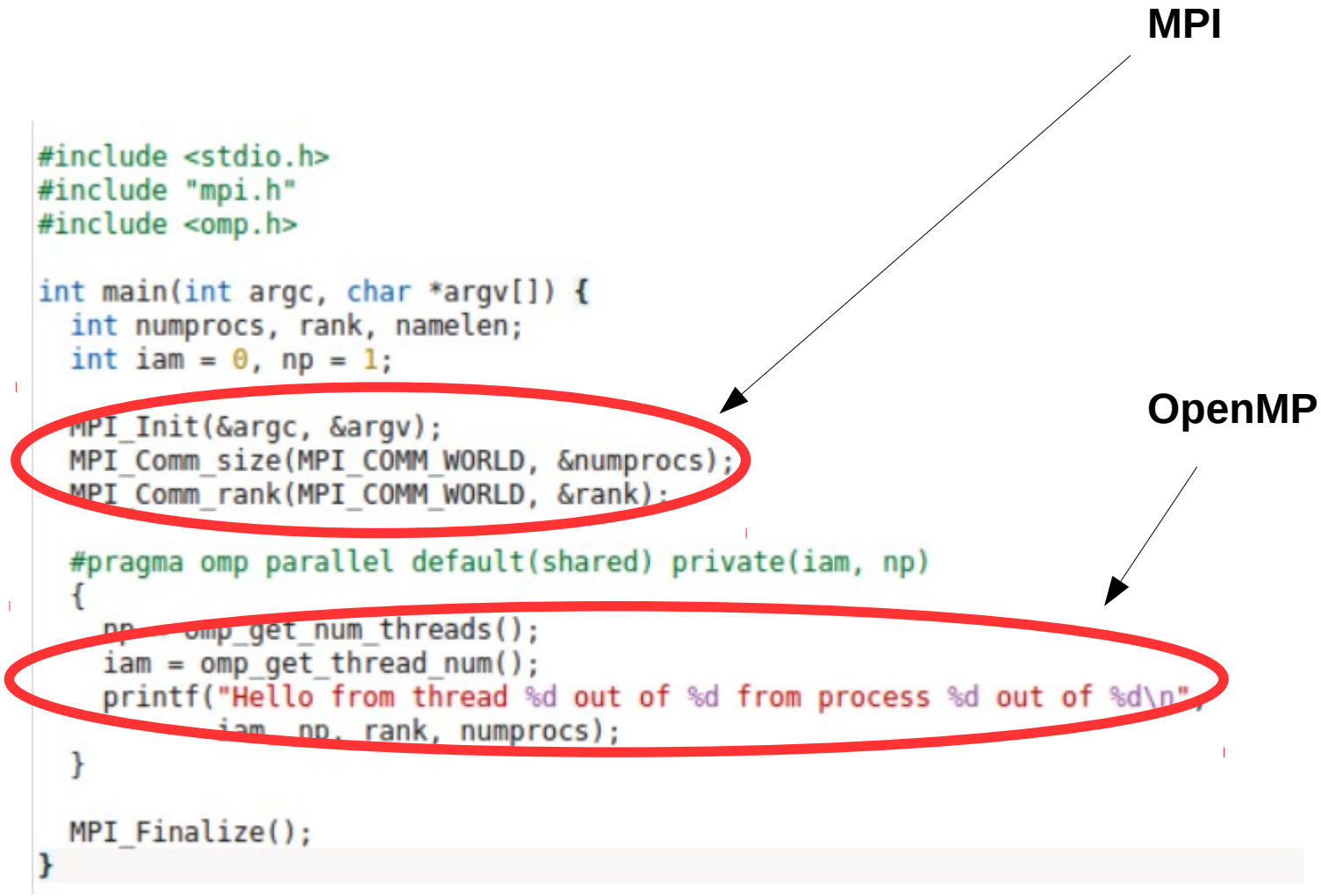
3. compile by typing:

> make

4. Experiment with different numbers of threads/MPI Processes

> export OMP_NUM_THREADS=4
> mpirun -np 2 ./1a.hello_world_hybrid.exec

Example

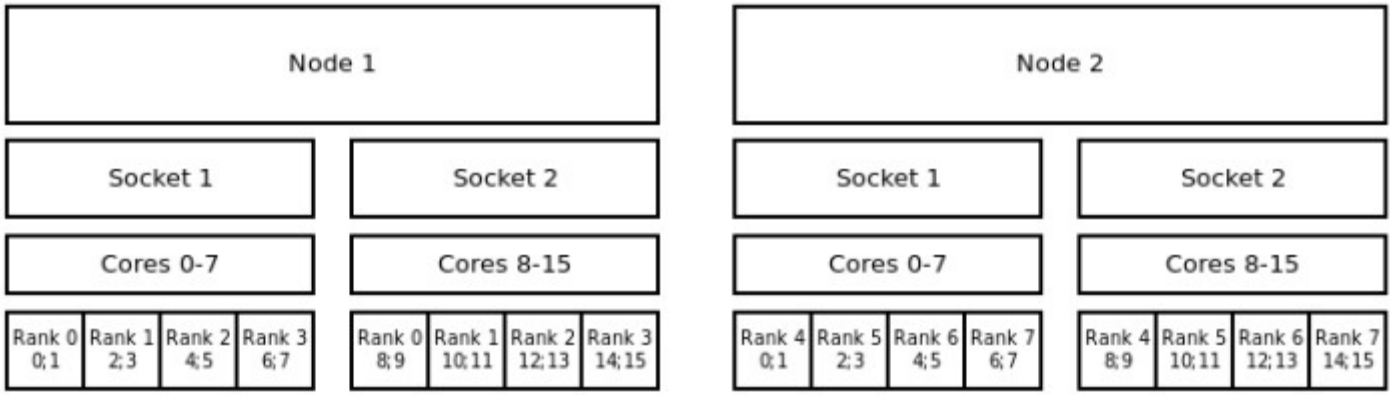



```c
#include <stdio.h>
#include "mpi.h"
#include <omp.h>

int main(int argc, char *argv[]) {
  int numprocs, rank, namelen;
  int iam = 0, np = 1;

  MPI_Init(&argc, &argv);
  MPI_Comm_size(MPI_COMM_WORLD, &numprocs);
  MPI_Comm_rank(MPI_COMM_WORLD, &rank);

  #pragma omp parallel default(shared) private(iam, np)
  {
    np = omp_get_num_threads();
    iam = omp_get_thread_num();
    printf("Hello from thread %d out of %d from process %d out of %d\n",
           iam, np, rank, numprocs);
  }

  MPI_Finalize();
}
```

Slurm with Hybrid Jobs

In the illustration below the default binding of a Hybrid-job is shown. In which 8 global ranks are distributed onto 2 nodes with 16 cores each. Each rank has 4 cores assigned to it.

```
#!/bin/bash
#SBATCH --nodes=2
#SBATCH --tasks-per-node=4
#SBATCH --cpus-per-task=4

export OMP_NUM_THREADS=4

srun --ntasks 8 --cpus-per-task $OMP_NUM_THREADS ./application
```



Example 2: Slurm on Midway

1. go to OSM_Lab/HPC_day4/code_day4/hybrid:

> cd OSM_Lab/HPC_day4/code_day4/hybrid

2. Have a look at the code

> vi submit_hybrid_midway.sh

3. compile by typing:

> make

4. Experiment with different numbers of nodes/threads/MPI Processes and look at the output.

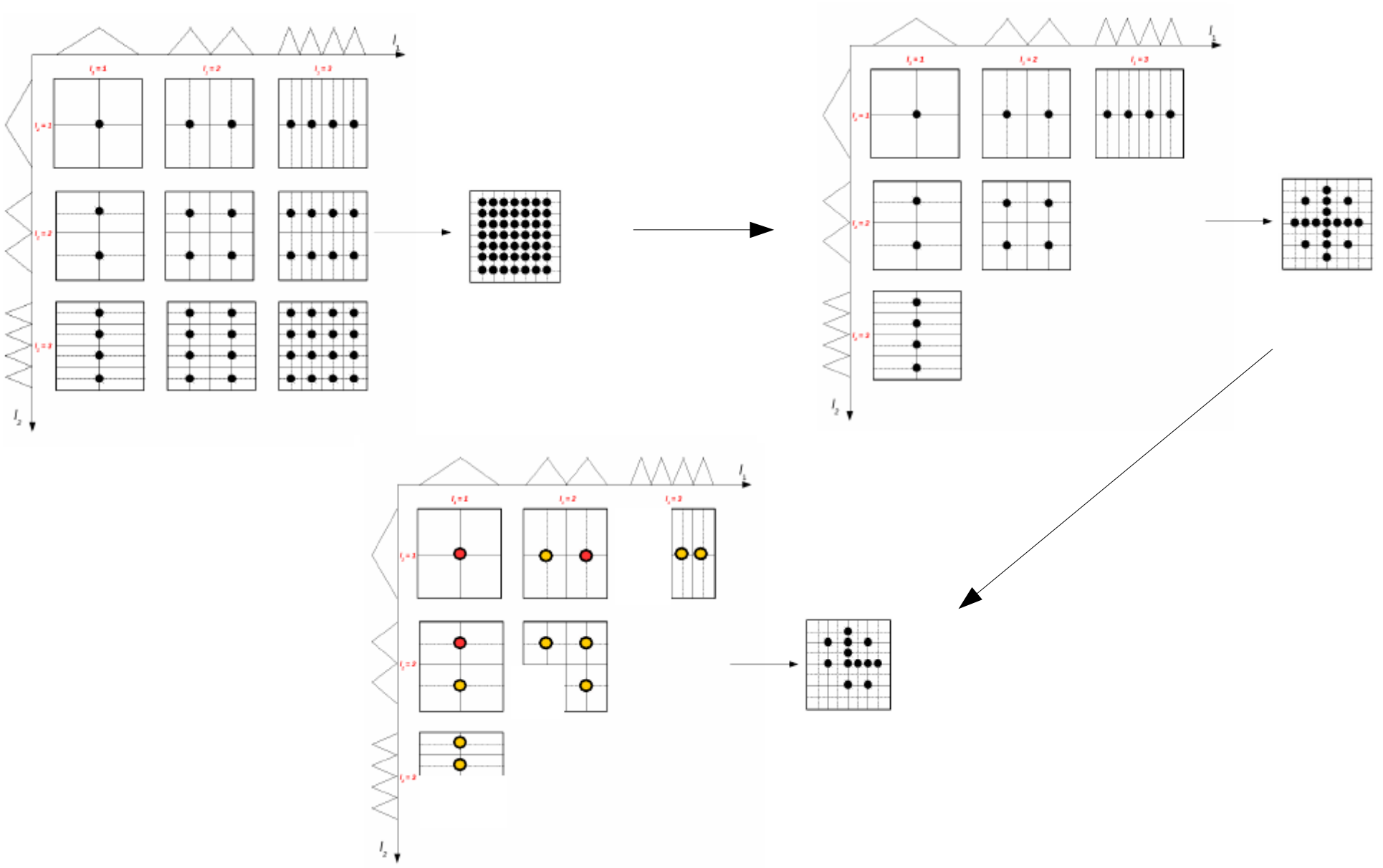
> sbatch submit_hybrid_midway.sh

Slurm – Hybrid

```
#!/bin/bash
# a sample job submission script to submit a hybrid MPI/OpenMP job to the sandyb
# partition on Midway1 please change the --partition option if you want to use
# another partition on Midway1

# set the job name to hello-hybrid
#SBATCH --job-name=hello-hybrid

# send output to hello-hybrid.out
#SBATCH --output=hello-hybrid.out

# this job requests 4 MPI processes
#SBATCH --ntasks=4


# and request 8 cpus per task for OpenMP threads
#SBATCH --cpus-per-task=8

# this job will run in the sandyb partition on Midway1
#SBATCH --partition=sandyb

# load the openmpi default module
module load openmpi

# set OMP_NUM_THREADS to the number of --cpus-per-task we asked for
export OMP_NUM_THREADS=$SLURM_CPUS_PER_TASK

# Run the process with mpirun. Notice -n is not required. mpirun will
# automatically figure out how many processes to run from the slurm options
mpirun ./1a.hello_world_hybrid.exec
```

Putting things together: Time Iteration, Adaptive Sparse Grids, HPC

Hybrid parallelism in Sparse grids



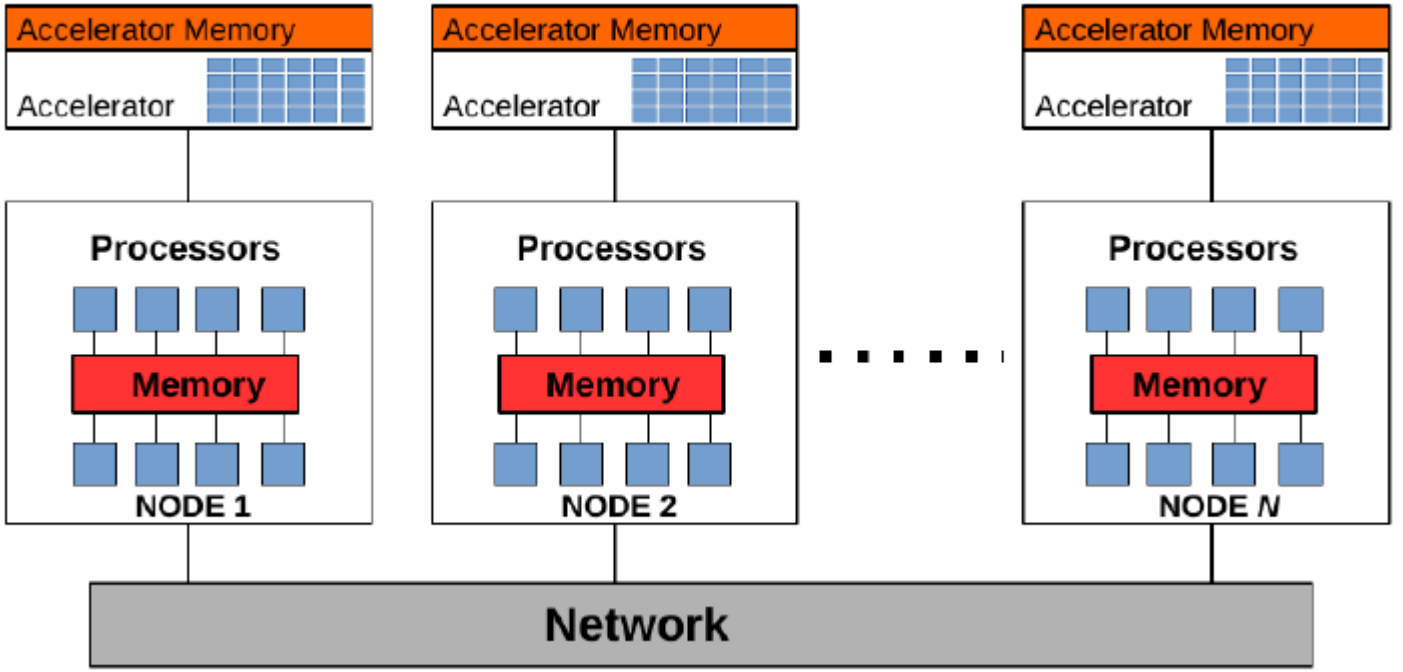
Algorithm for time iteration & SG

Scheidegger et al. (2017)

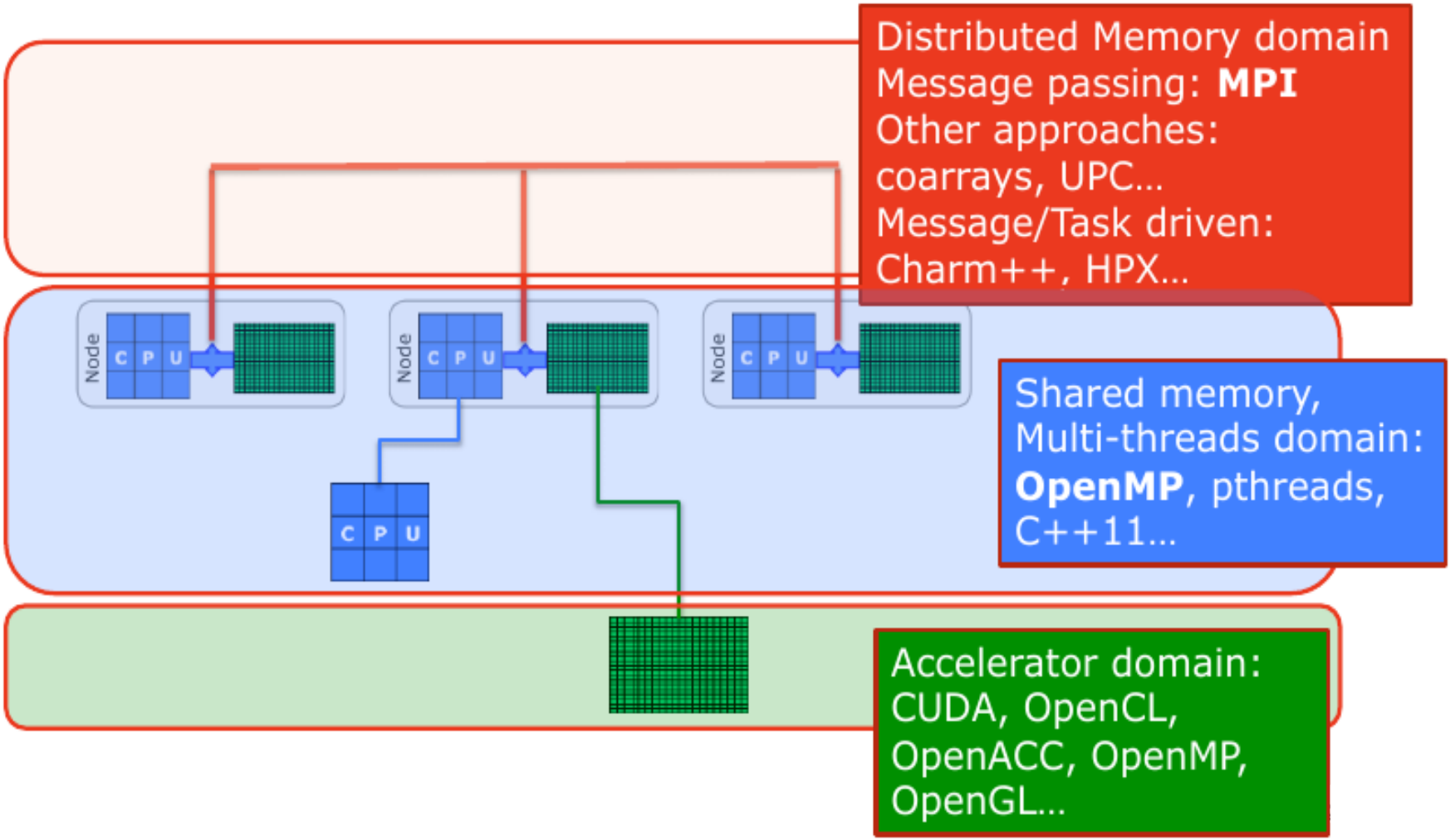
Data: Initial guess $p_{next} = (p_{next}(1), \ldots, p_{next}(N_s = 16)$ for next period's policy function. Approximation accuracy $\bar{\eta}$. Maximal refinement level L_{max}. Starting refinement level $L_0 \leq L_{max}$. Refinement threshold ϵ.
Result: The (approximate) equilibrium policy function $p = (p(1), \ldots, p(N_s = 16))$.
while $\eta > \bar{\eta}$ **do**
  Set $z = 1$.
  for $z \leq N_s$ **do**
    Set $l = 1$, set $G(z) \subset S(z)$ to be the level 1 grid on $S(z)$, and set $G_{old}(z) = \emptyset, G_{new}(z) = \emptyset$.
    while $G(z) \neq G_{old}(z)$ **do**
      for $g(z) \in G(z) \setminus G_{old}(z)$ **do**
        Compute the optimal policies $p(g(z))$ by evaluating (5) to (15) given next period's policy p_{next}.
        Define the policy $\tilde{p}(g((z)))$ by interpolating $\{p(g(z))\}_{g(z) \in G_{old}(z)}$.
        if $(l < L_{max}$ *and* $\|p(g(z)) - \tilde{p}(g(z))\|_\infty > \epsilon)$ *or* $l < L_0$, **then**
          Add the neighboring points (*sons*) of $g(z)$ to $G_{new}(z)$.
        end
      end
      Set $G_{old}(z) = G(z)$, set $G = G_{old}(z) \cup G_{new}(z)$, set $G_{new}(z) = \emptyset$, and set $l = l + 1$.
    end
    Define the policy function $p(z)$ as the sparse grid interpolation of $\{p(g(z))\}_{g(z) \in G(z)}$.
    Calculate (an approximation for) the error within a state:
    $\eta(z) = \|p(z) - p_{next}(z)\|$. Set $p_{next}(z) = p(z)$.
    set $z = z + 1$.
  end
  error: $\eta = \max(\eta(1), \ldots, \eta(N_s))$
end

Algorithm 1: Overview of the crucial steps of the time iteration algorithm.

Recall – Today's HPC systems



Overall picture of programming models



(Slide from C. Gheller)

Parallel time iteration/DP algorithm

Brumm et al. (2015), Brumm & Scheidegger (2017)

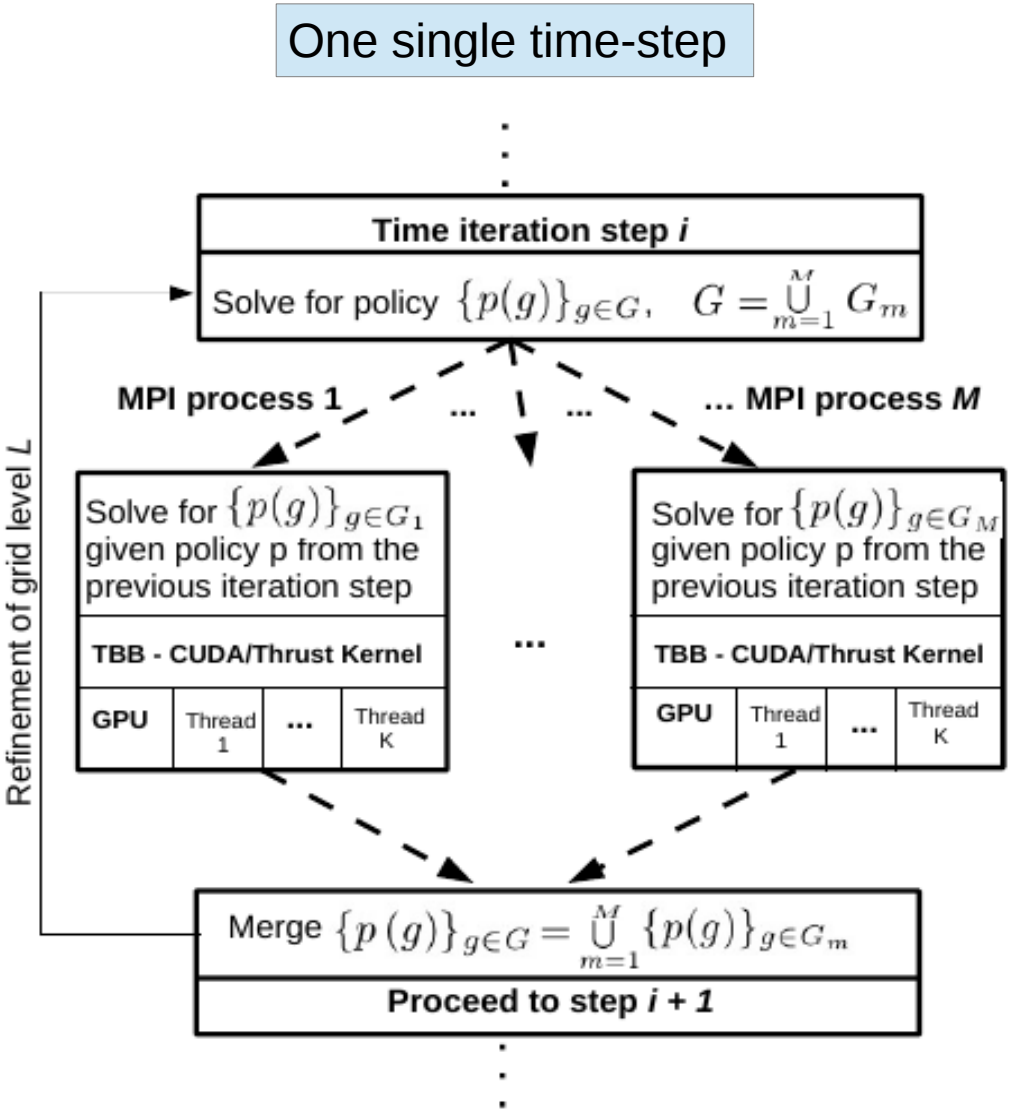
-Our implementation:
Hybrid parallel
(MPI & Intel TBB & GPU (CUDA/THRUST)).

-newly generated points are distributed via MPI

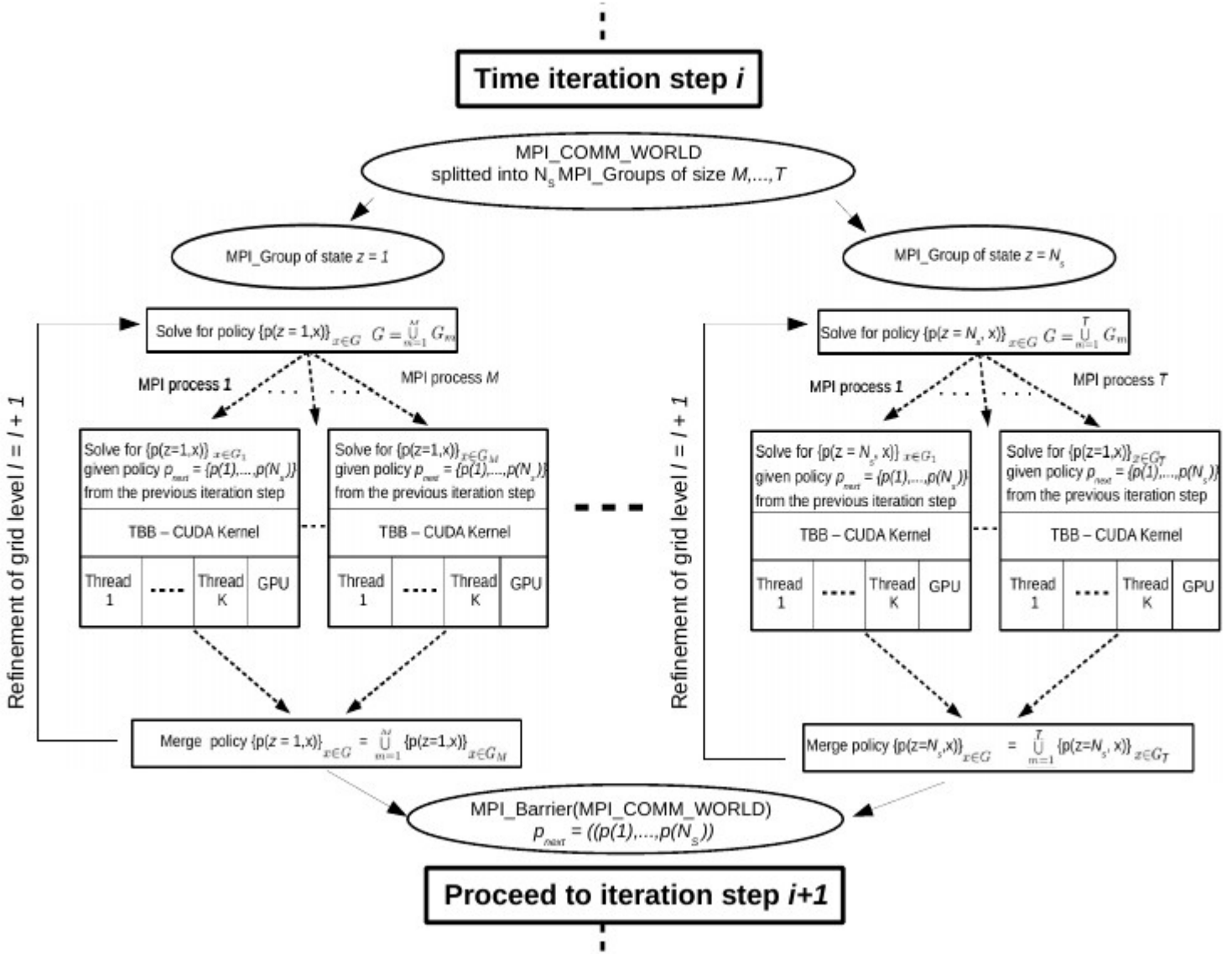
Solve optimizations/ nonlinear equations locally
(e.g. IPOPT (Waechter & Biegler (2006)).

In parallel: `messy' !

→ policy from previous iteration visible on all MPI processes.
→ we have to ensure some sort of `load balancing'.
→ **Now a lot better with TBB**

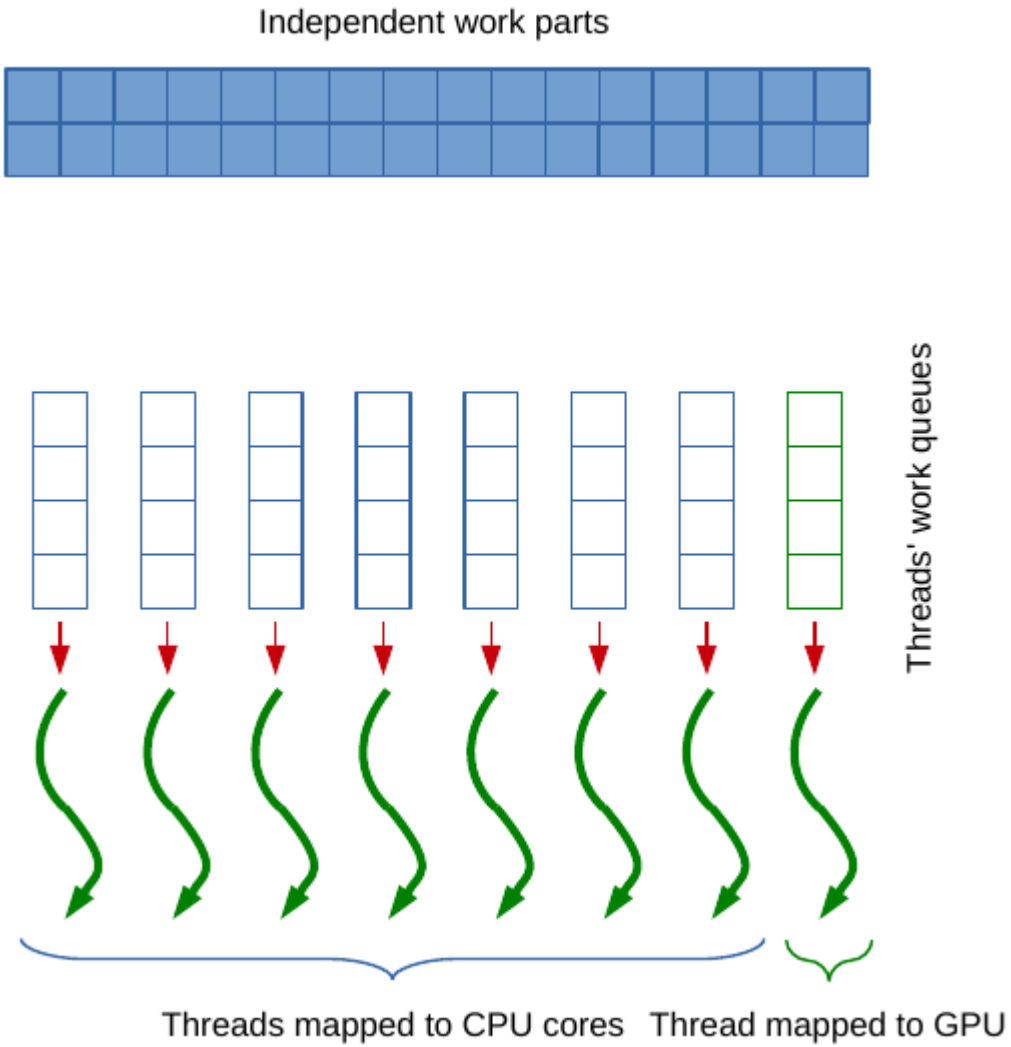


With discrete states



Intel® Threading Building Blocks (TBB)

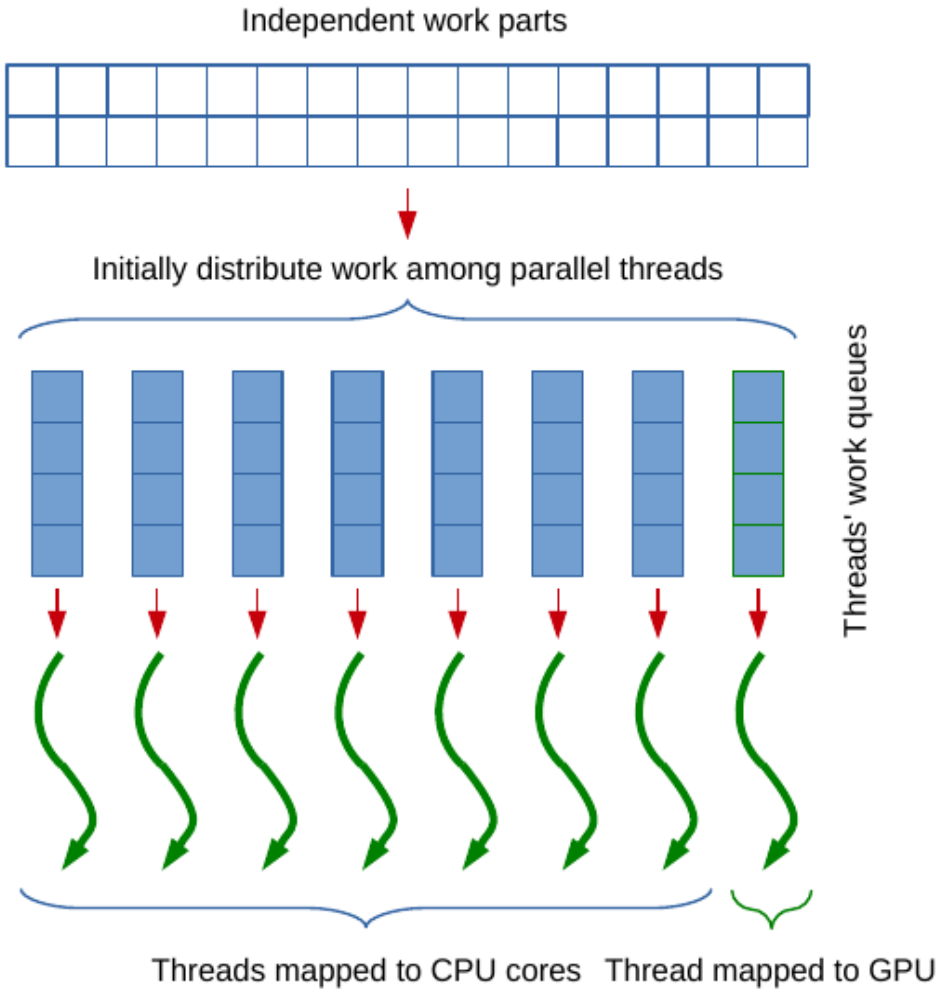
-TBB maps different threads, similar to OpenMP.



Intel® Threading Building Blocks (TBB)

-TBB maps different threads, similar to OpenMP.

-Every thread is initially assigned an equal logical queue of tasks.



Intel® Threading Building Blocks (TBB)

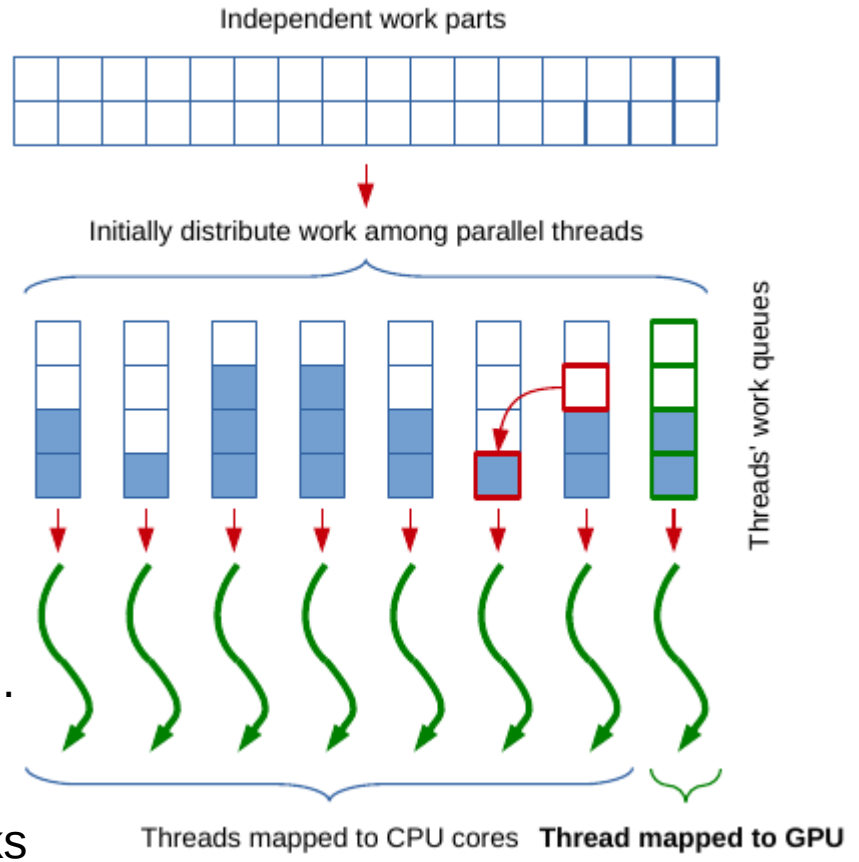
-TBB maps different threads, similar to OpenMP.

-Every thread is initially assigned an equal logical queue of tasks.

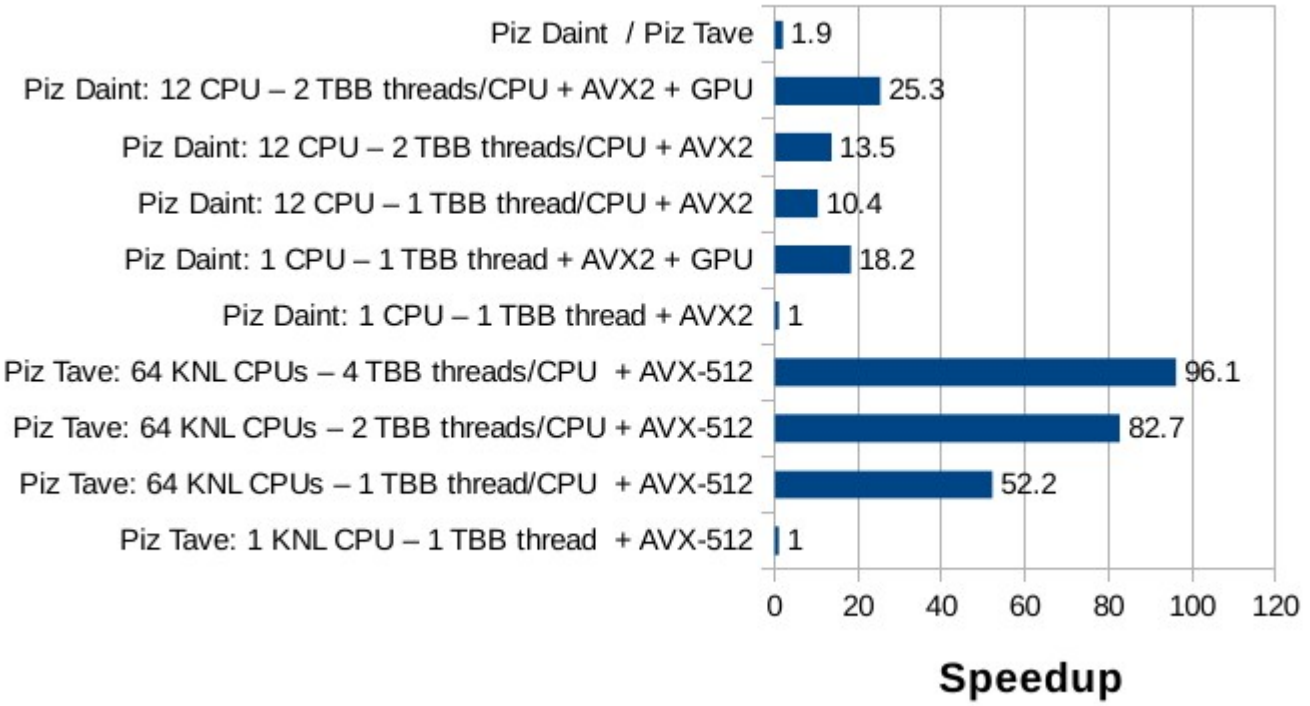
-However, different tasks may be processed faster or slower, due to differences between tasks and/or compute cores

-TBB approach to work balancing: once one thread runs out of tasks, **“steal” a task from another thread, which makes slower progress**.

-We map one extra thread onto **GPU**
→ **CPU** cores and **GPU** process interpolation tasks together.

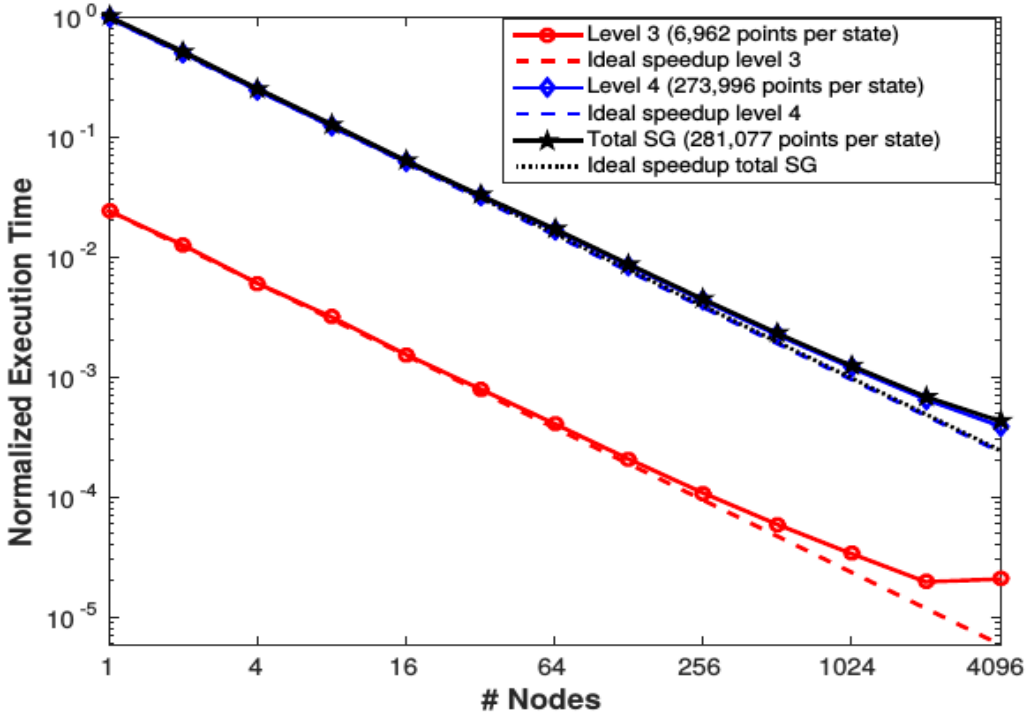


Strong scaling – 1 node



Strong scaling – intra-node

Scheidegger et al. (2017)



- Annually calibrated OLG model.
- 16 discrete states (stochastic tax rates on labor and capital).
- solve this model in few hours.

Figure 6: Strong scaling on Piz Daint for an OLG model using 4 levels of grid refinements, 16 discrete states, and $16 \cdot 281,077 = 4,497,232$ points and $265,336,688$ unknowns in total. "Total SG" shows the entire, normalized simulation time up to $4,096$ nodes. We also show normalized execution times for the computational sub-components on different levels, e.g., for level 3 using 6.962 points. Dashed and dotted lines show the ideal speedup.

Time to soluton

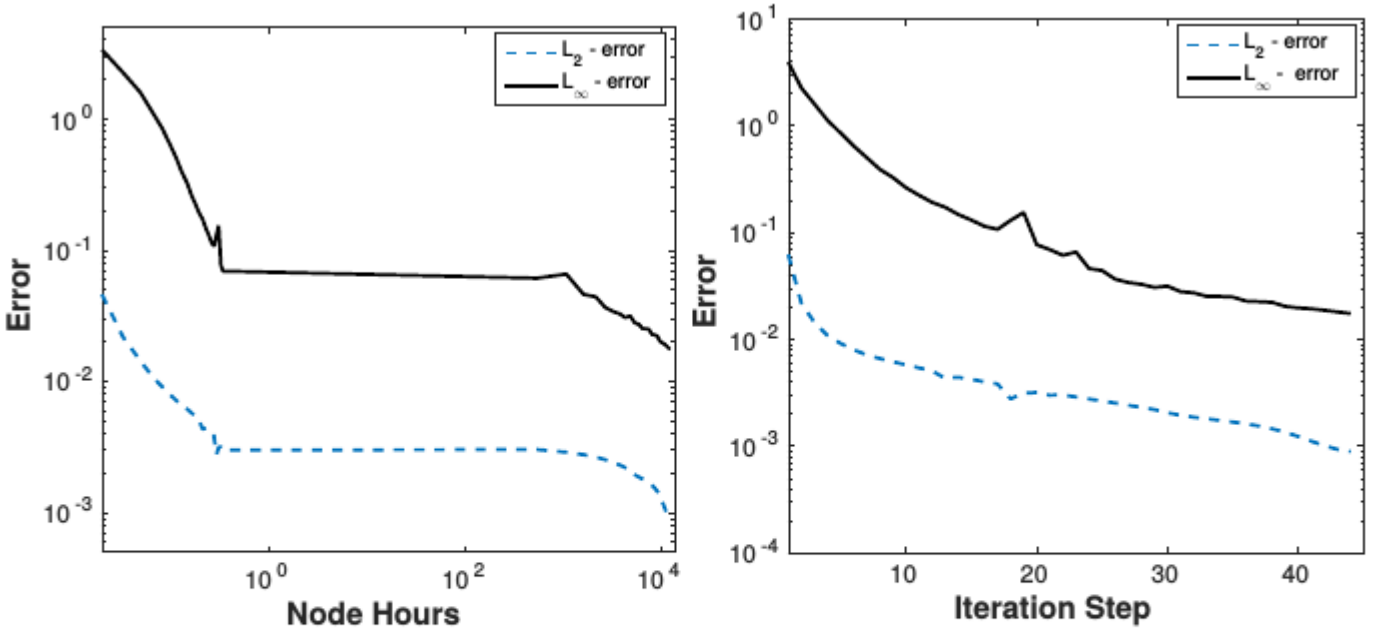


Figure 7: Comparison of the L_2 and L_∞–error for adaptive sparse grid solutions of the 59-dimensional OLG model as a function of compute time or iterations spent on Piz Daint.

Questions?

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