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Hybrid parallel programming

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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

Outline

Hybrid parallelism in general

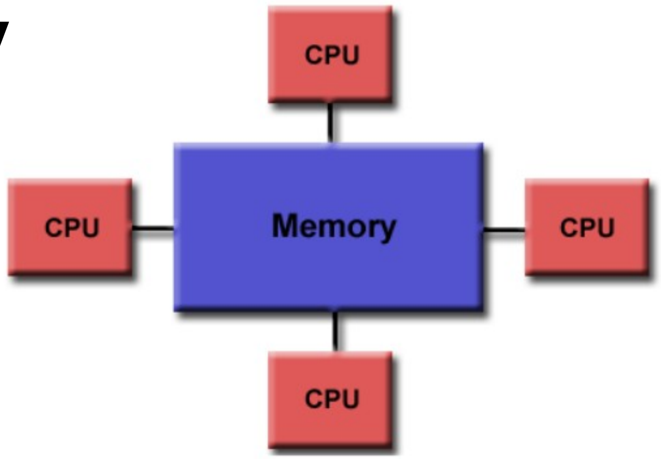
- Recap hardware & programming models
- Merging OpenMP & MPI
- “Hello World” in hybrid

Putting things together:

- Time Iteration, Adaptive Sparse Grids, HPC

Shared memory systems – OpenMP

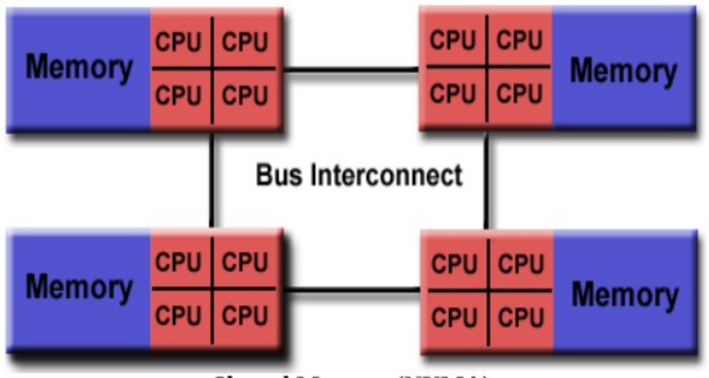
- **Process can access same GLOBAL memory**



Shared Memory (UMA)

- **Uniform Memory Access (UMA) model**
  - Access time to memory is uniform.
  - Local cache, all other peripherals are shared.

- **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.



Shared Memory (NUMA)

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

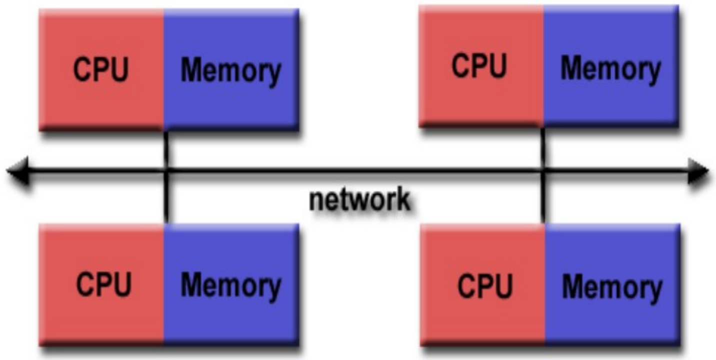
Distributed-memory parallel programming – MPI

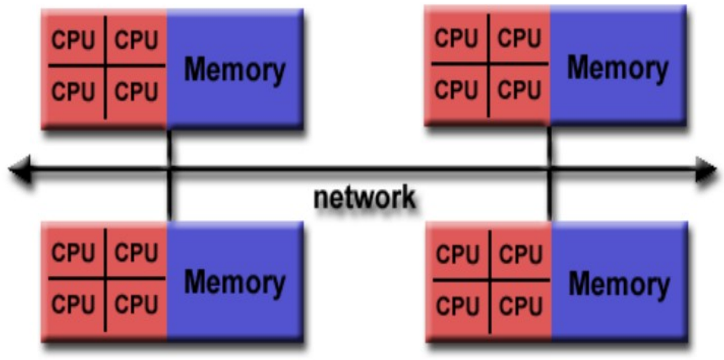
- We need to use explicit message passing, i.e., communication between processes:
  → Most tedious and complicated but also the most flexible parallelization method.

- 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)**.



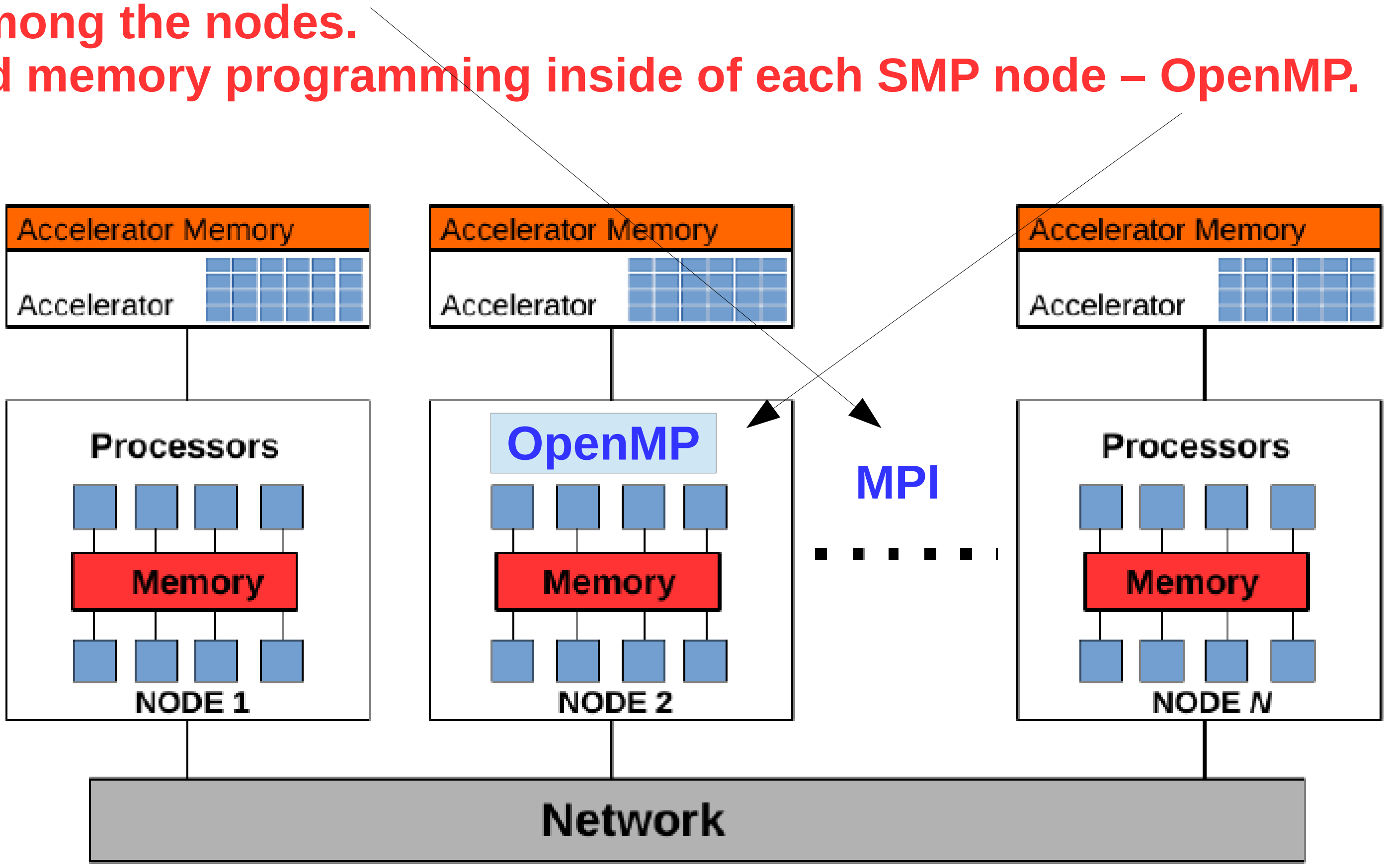


Today's HPC systems

- 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**:

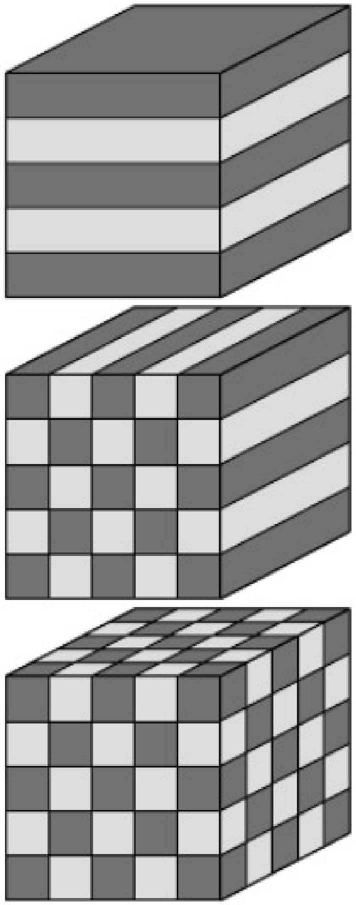
→ for 8/16/32/64/...ranks per multi-core node, this can have scaling problems with many nodes/MPI ranks.

→ **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"

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

"Poles"

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

"Cubes"

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

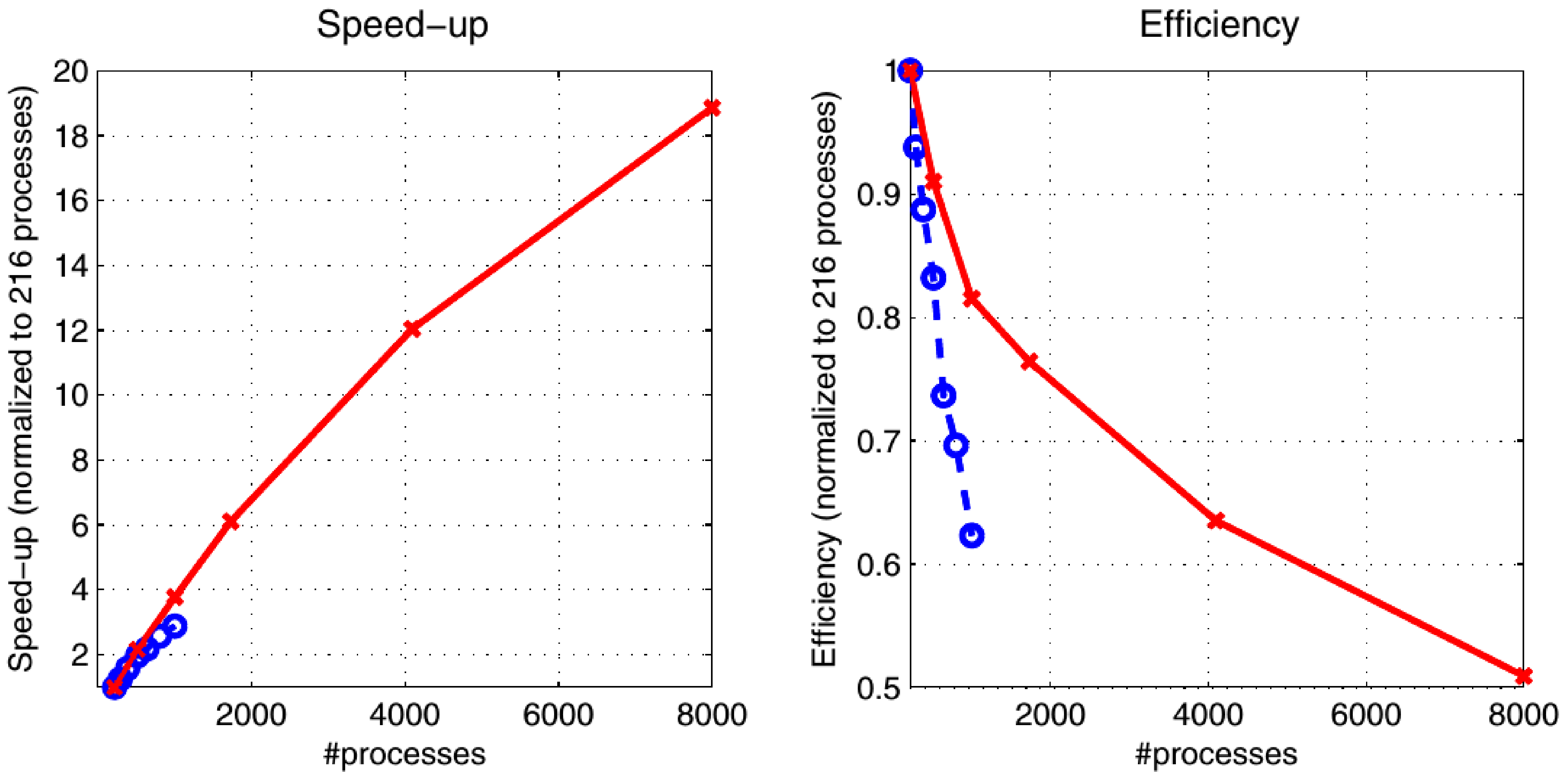
Figure 10.9: 3D domain decomposition of a cubic domain of size L^3 (strong scaling) and periodic boundary conditions: Per-process communication volume $c(L,N)$ for a single-site data volume w (in bytes) on N processes when cutting in one (top), two (middle), or all three (bottom) dimensions.

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

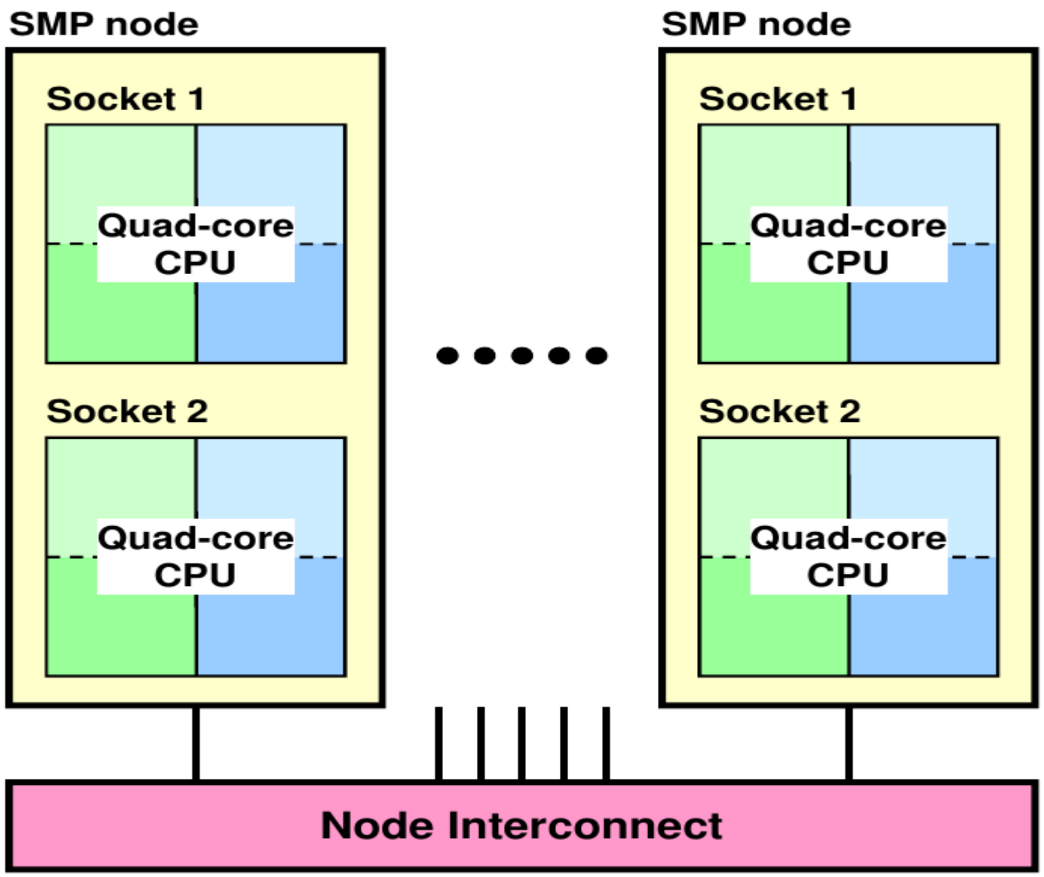
- How many threads (i.e., cores) per MPI process?
  → Too few threads, too much memory consumption

- 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)

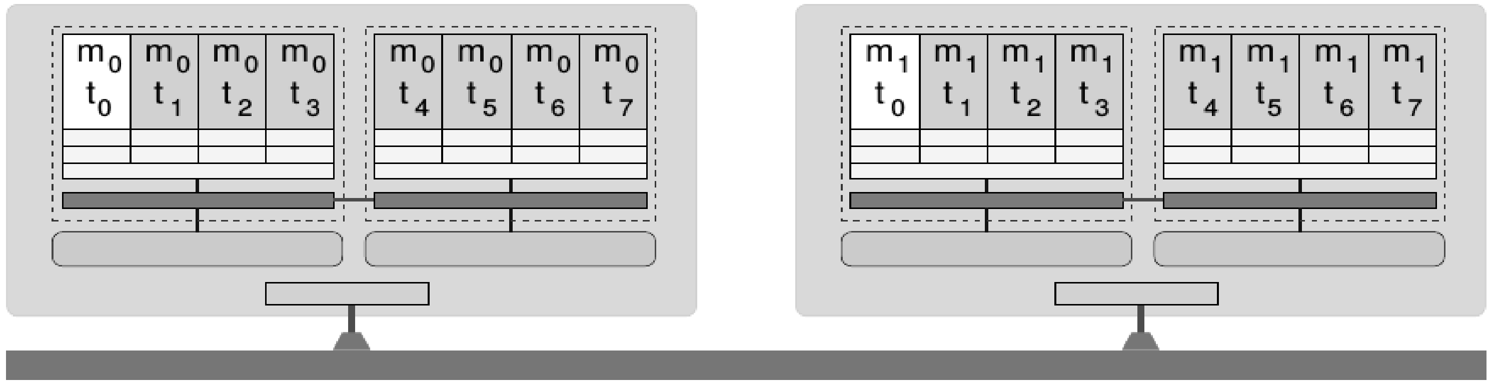


Figure 11.3: Mapping a single MPI process with eight threads to each node.

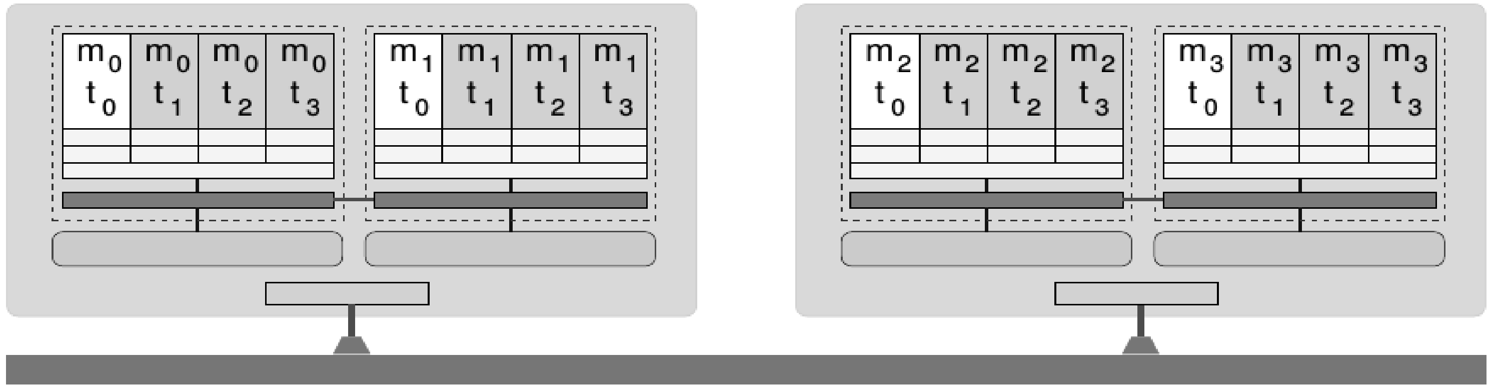


Figure 11.4: Mapping a single MPI process with four threads to each socket (L3 group or locality domain).

From Hager & Wellein (2011)

Mapping (3)

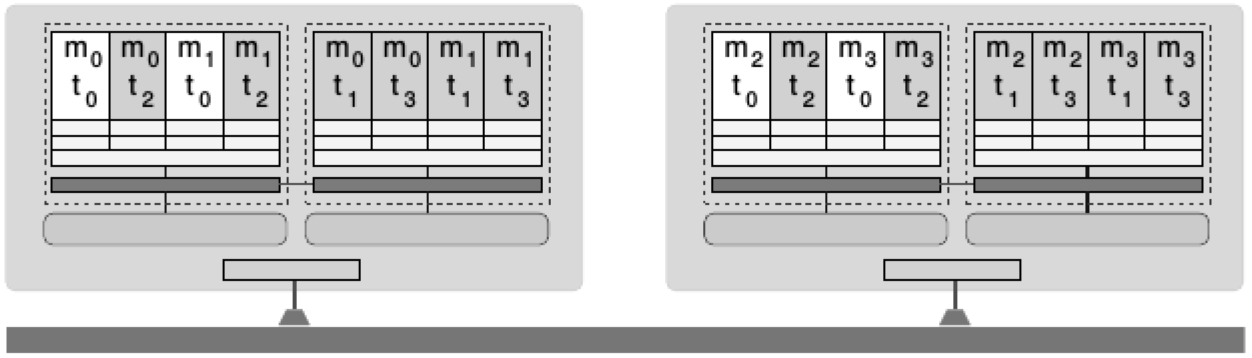


Figure 11.5: Mapping two MPI processes to each node and implementing a round-robin thread distribution.

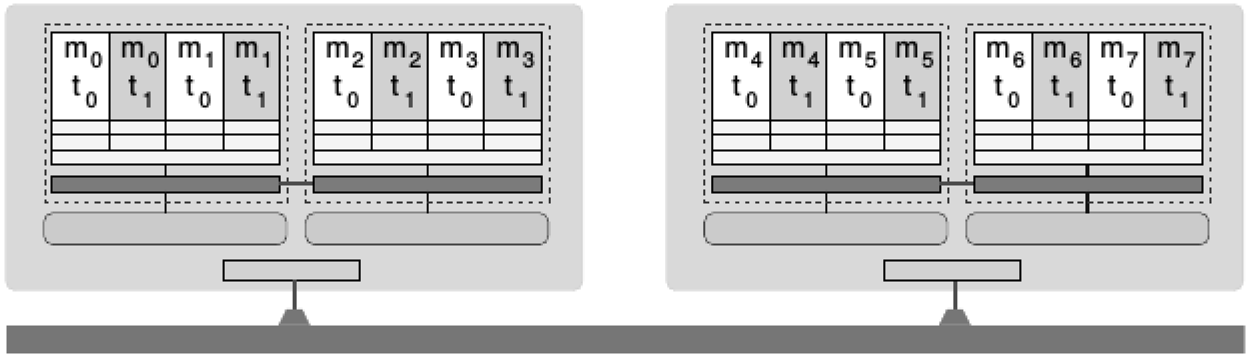


Figure 11.6: Mapping two MPI processes with two threads each to a single socket.

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 OSE2019/day4/code_day4/hybrid:

```
> cd OSM2019/day4/code_day4/hybrid
```

2. Have a look at the code

```
> vi 1a.hello_world_hybrid.cpp
```

3. compile by typing:

```
> make
```

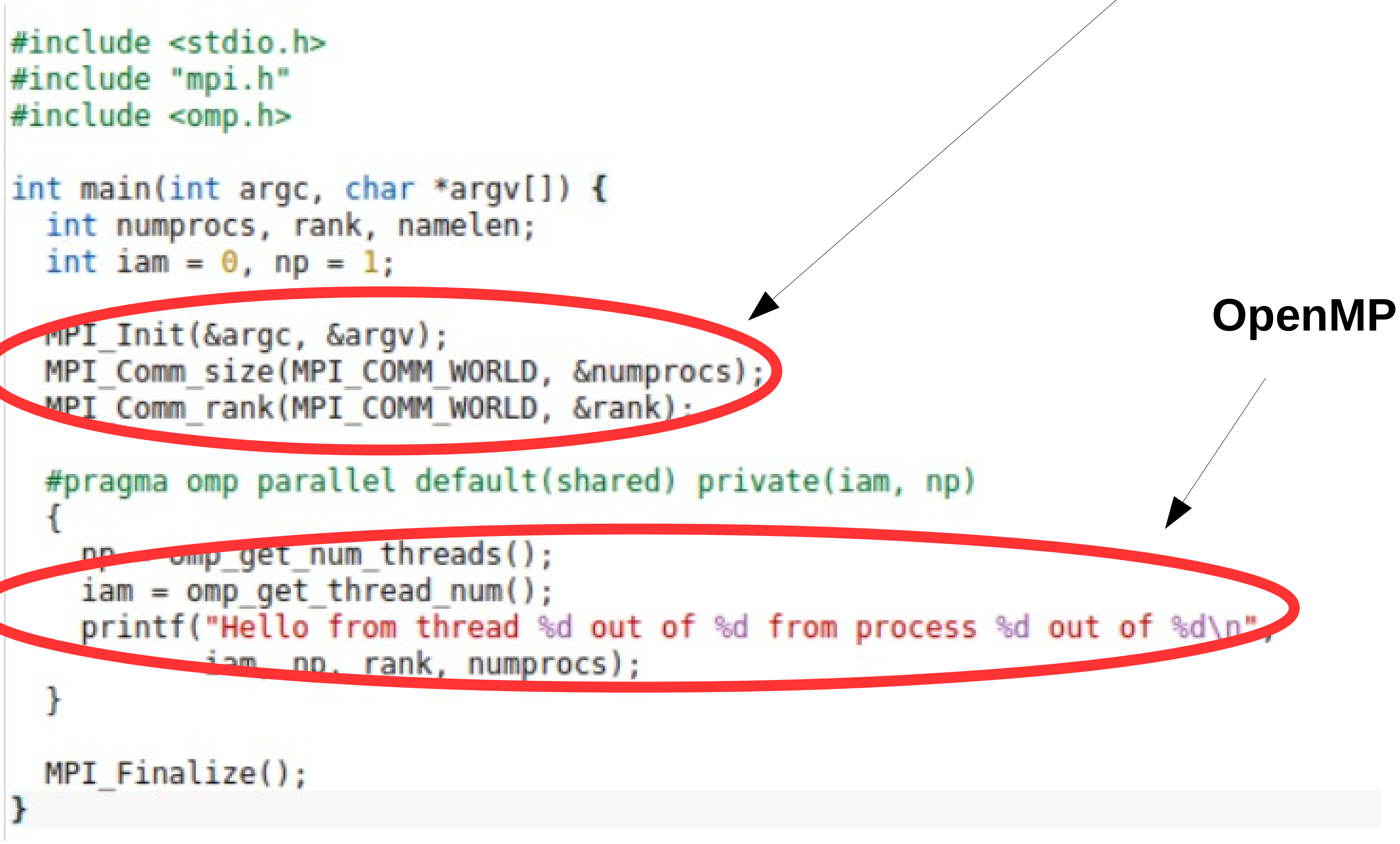
4. Experiment with different numbers of threads/MPI Processes

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

Example

MPI

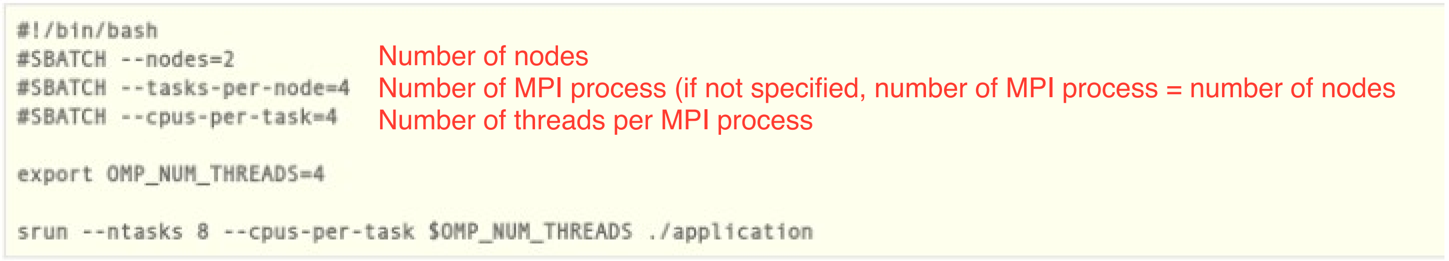
OpenMP



```
#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();
}
```

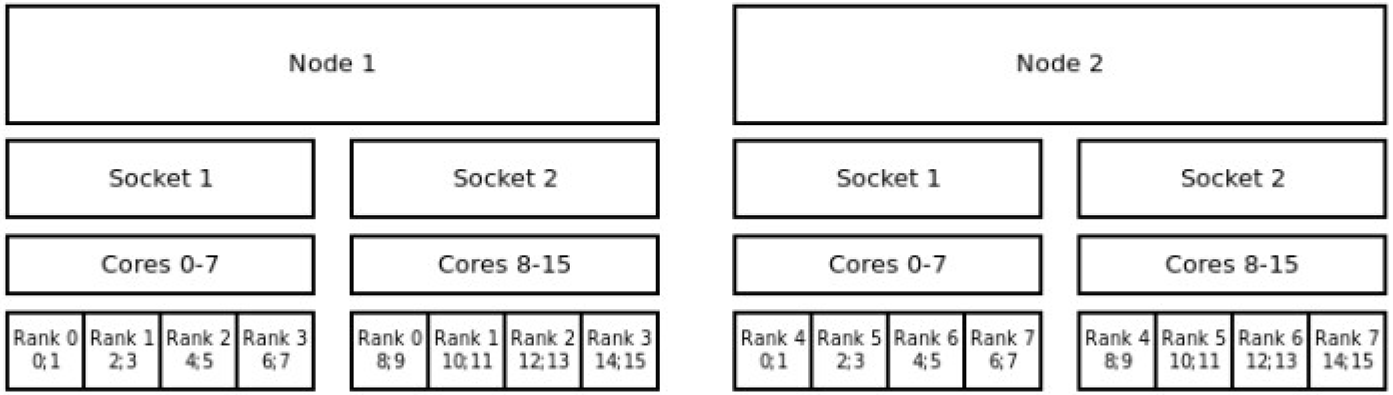
Slurm with Hybrid Jobs

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
```

Number of nodes
Number of MPI process (if not specified, number of MPI process = number of nodes
Number of threads per MPI process



Example 2: Slurm on Midway

1. go to OSE2019/day4/code_day4/hybrid:

```
> cd OSE2019/day4/code_day4/hybrid
```

2. Have a look at the code

```
> vi submit_hybrid_midway.sh
```

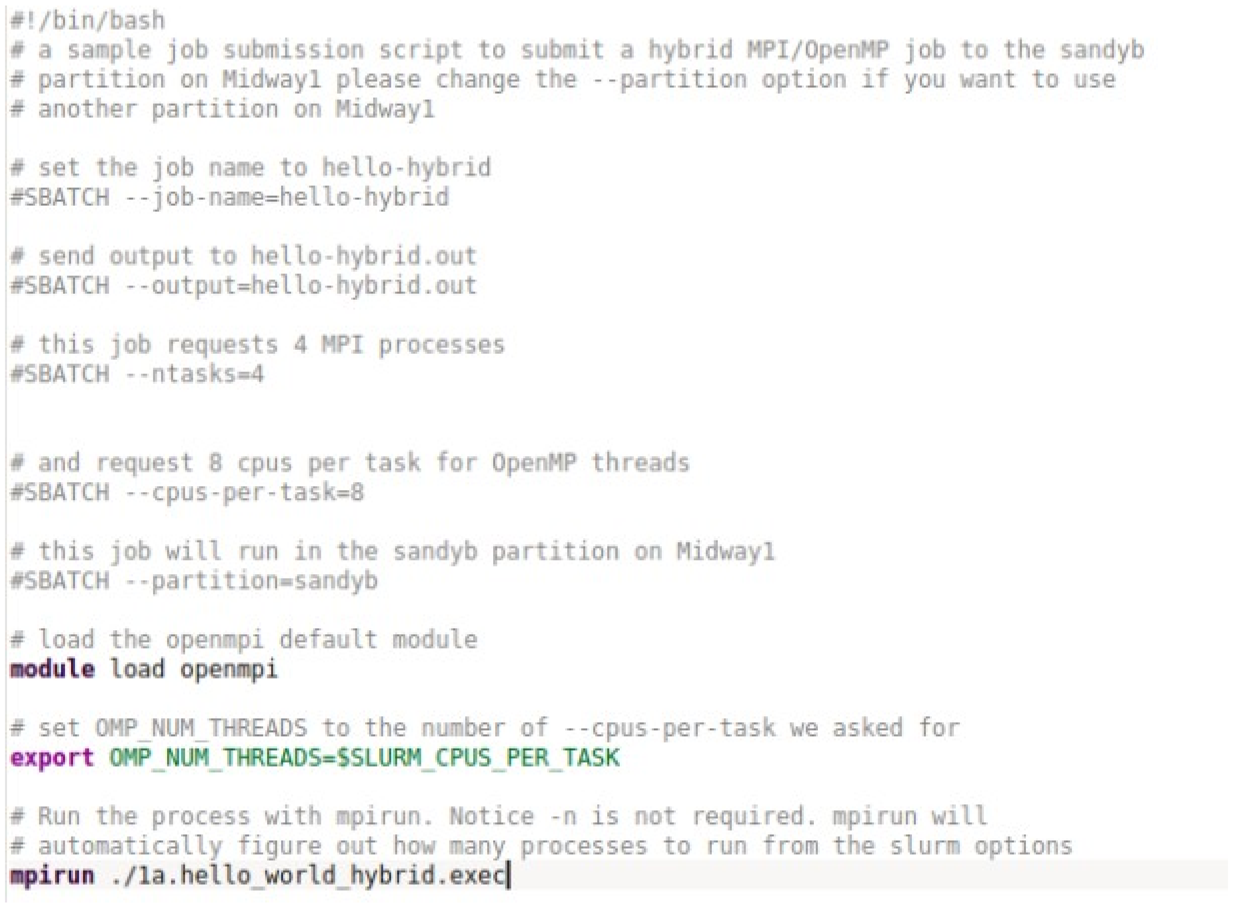
3. compile by typing:

```
> make
```

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

```
> sbatch submit_hybrid_midway.sh
```

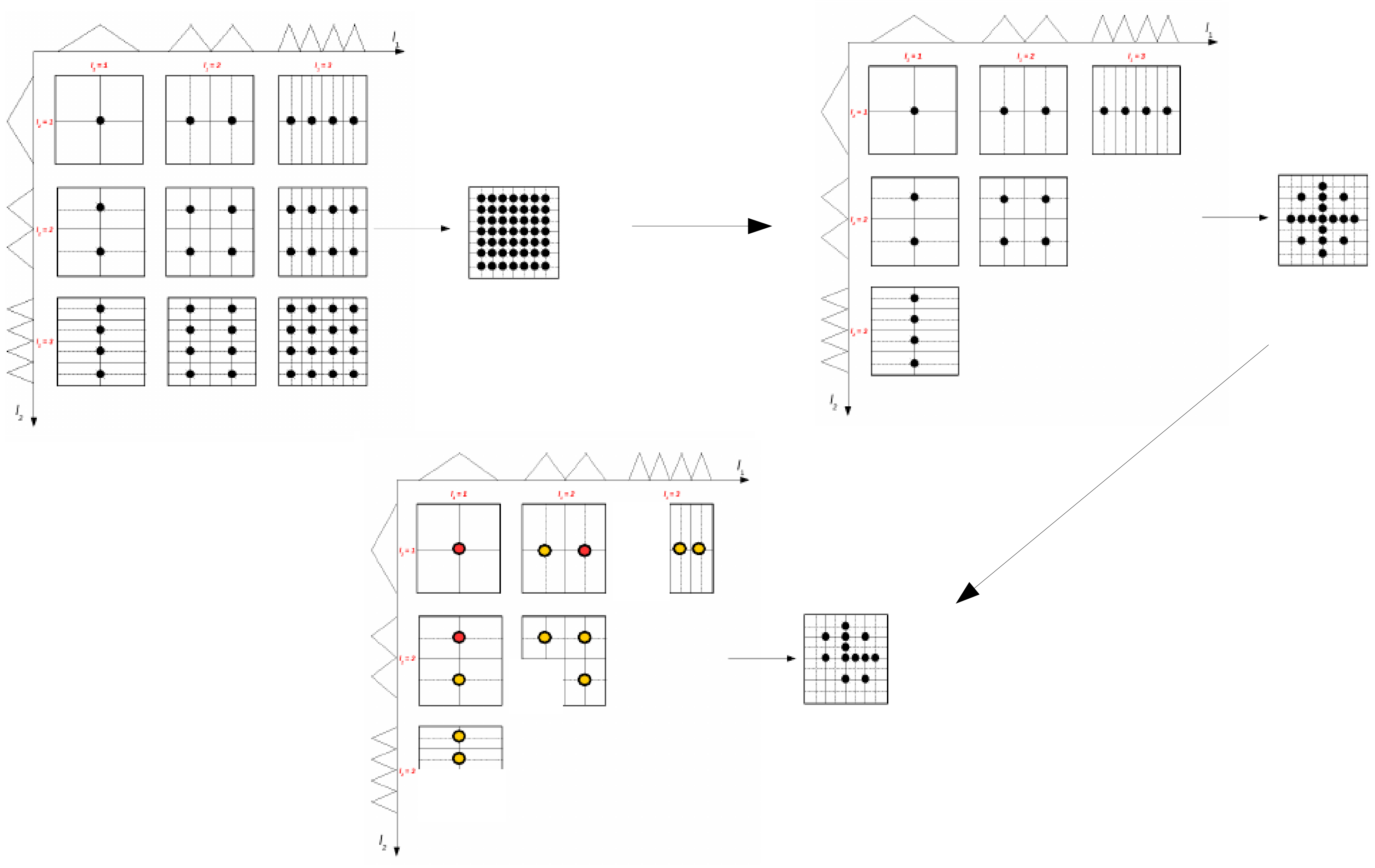
Slurm – Hybrid



```
#!/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

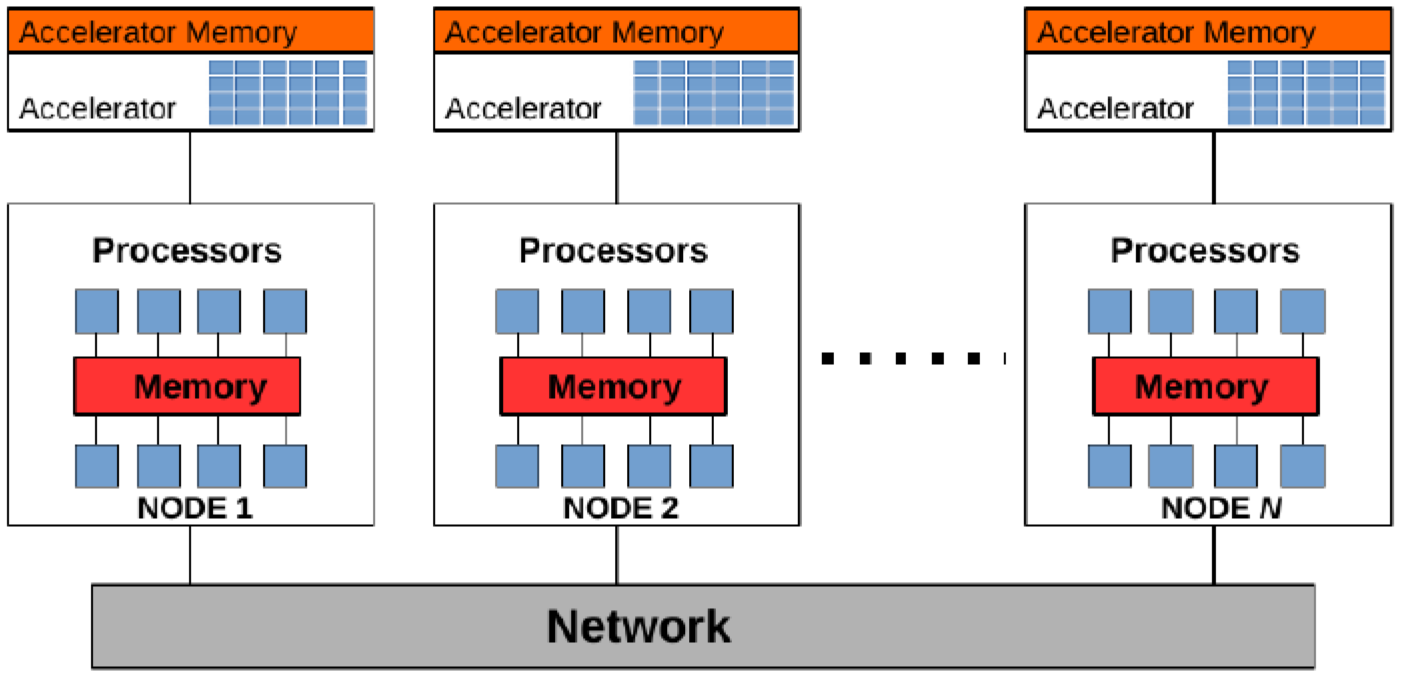
Scheidegger et al. (2017)

```
Data: Initial guess $p_{next} = (p_{next}(1), \dots, p_{next}(N_s = 16)$ 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 $\epsilon$.
Result: The (approximate) equilibrium policy function $p = (p(1), \dots, p(N_s = 16))$.
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: $\eta = \max(\eta(1), \dots, \eta(N_s))$
end
```

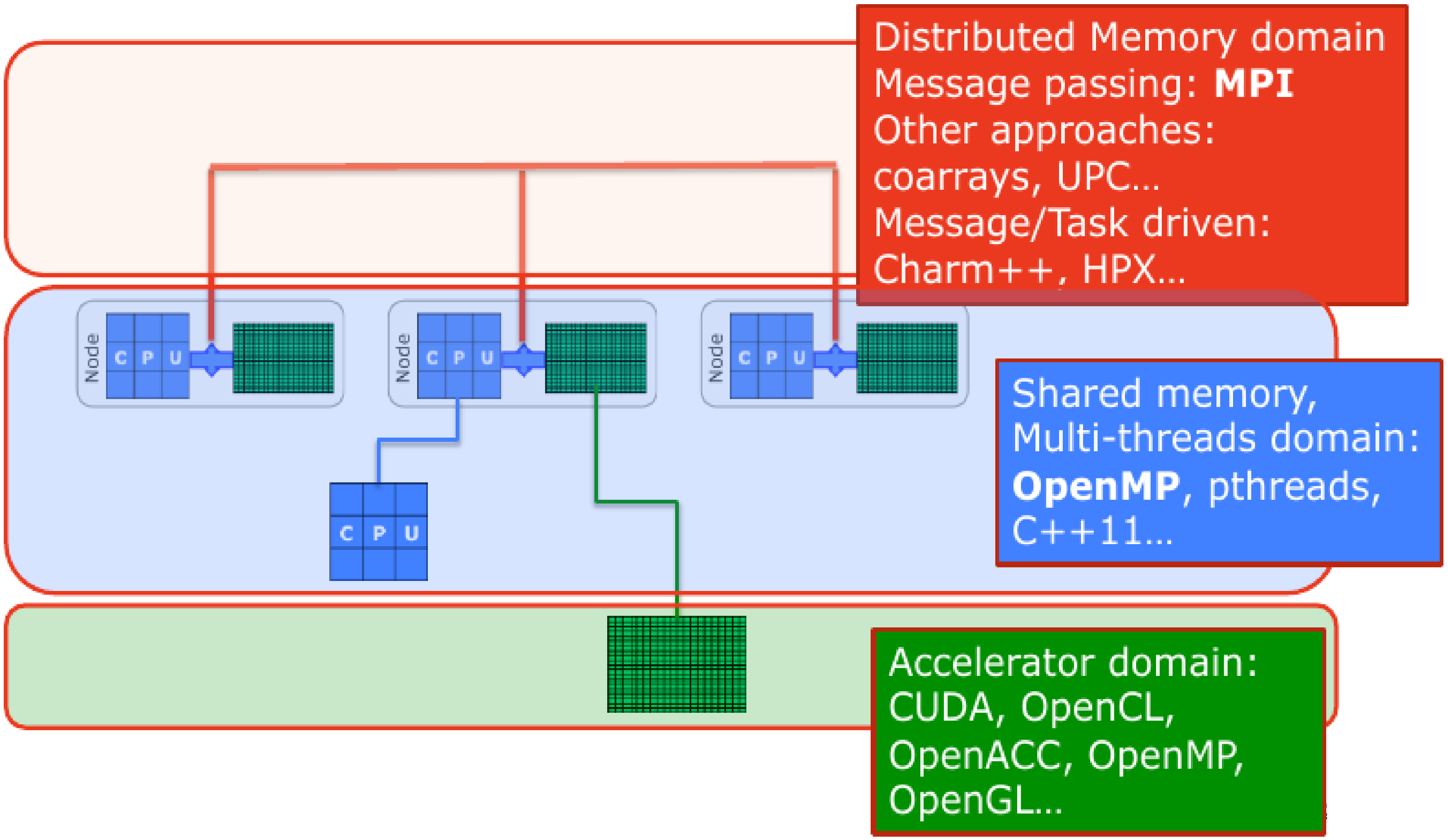
First: what is independent? States, say request 160 nodes, so per state gets 10 nodes.
Second: with in first layer, what is independent? Each grid point, say 1000 grid points per state,
say if there are 10 CPUs per node, so each CPU gets 10 points to compute.
Must code generally so that the points are (almost) evenly spread after adaptive sparse steps.

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

Recall – Today's HPC systems



Overall picture of programming models



Distributed Memory domain
Message passing: **MPI**
Other approaches:
coarrays, UPC...
Message/Task driven:
Charm++, HPX...

Shared memory,
Multi-threads domain:
OpenMP, pthreads,
C++11...

Accelerator domain:
CUDA, OpenCL,
OpenACC, OpenMP,
OpenGL...

(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)).

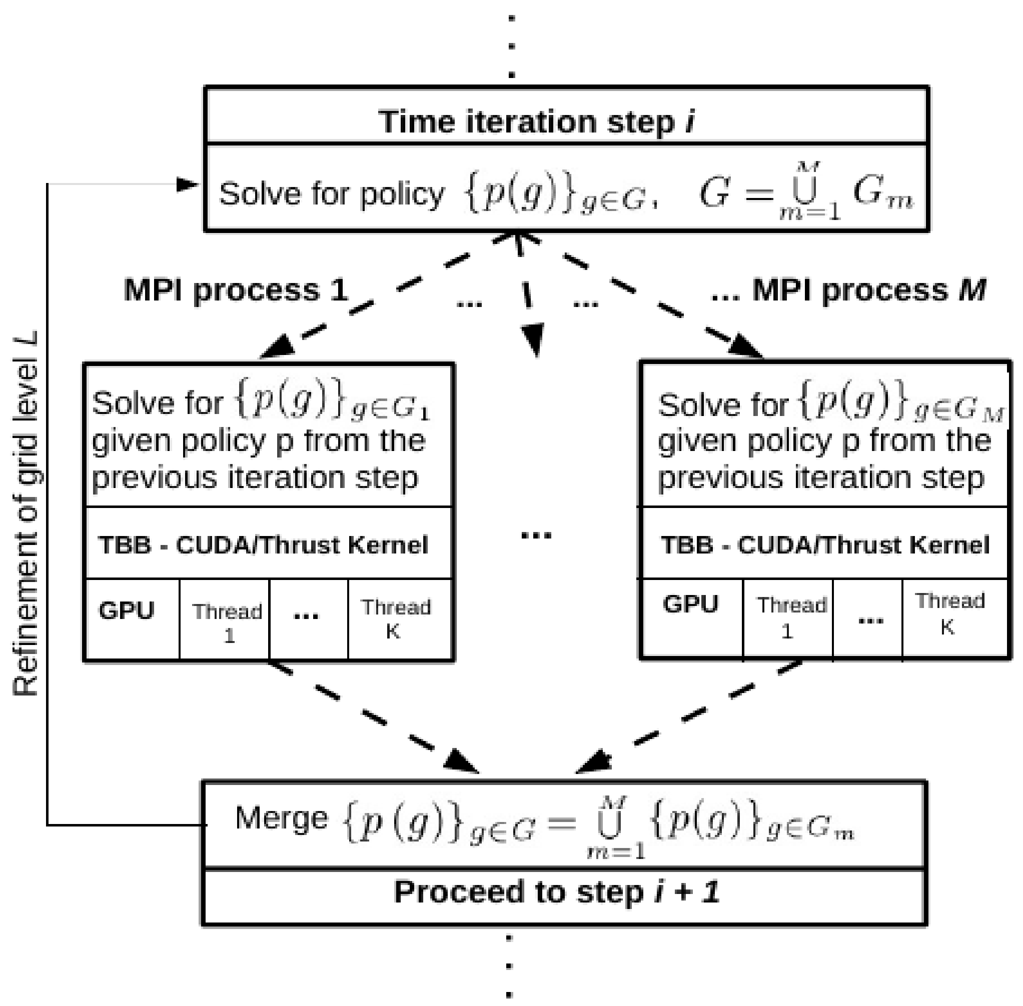
-newly generated points are distributed via MPI

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

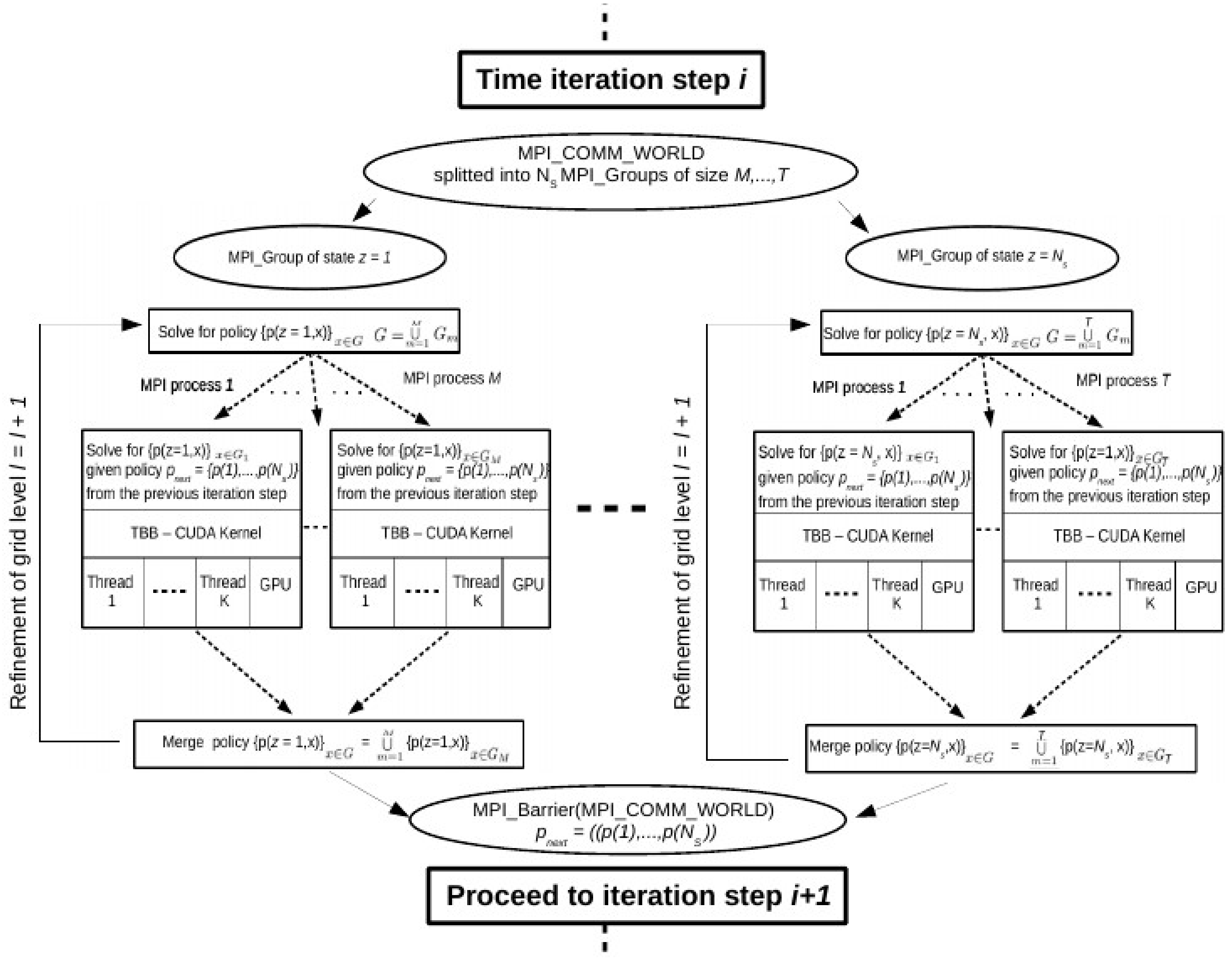
In parallel: `messy' !

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

One single time-step

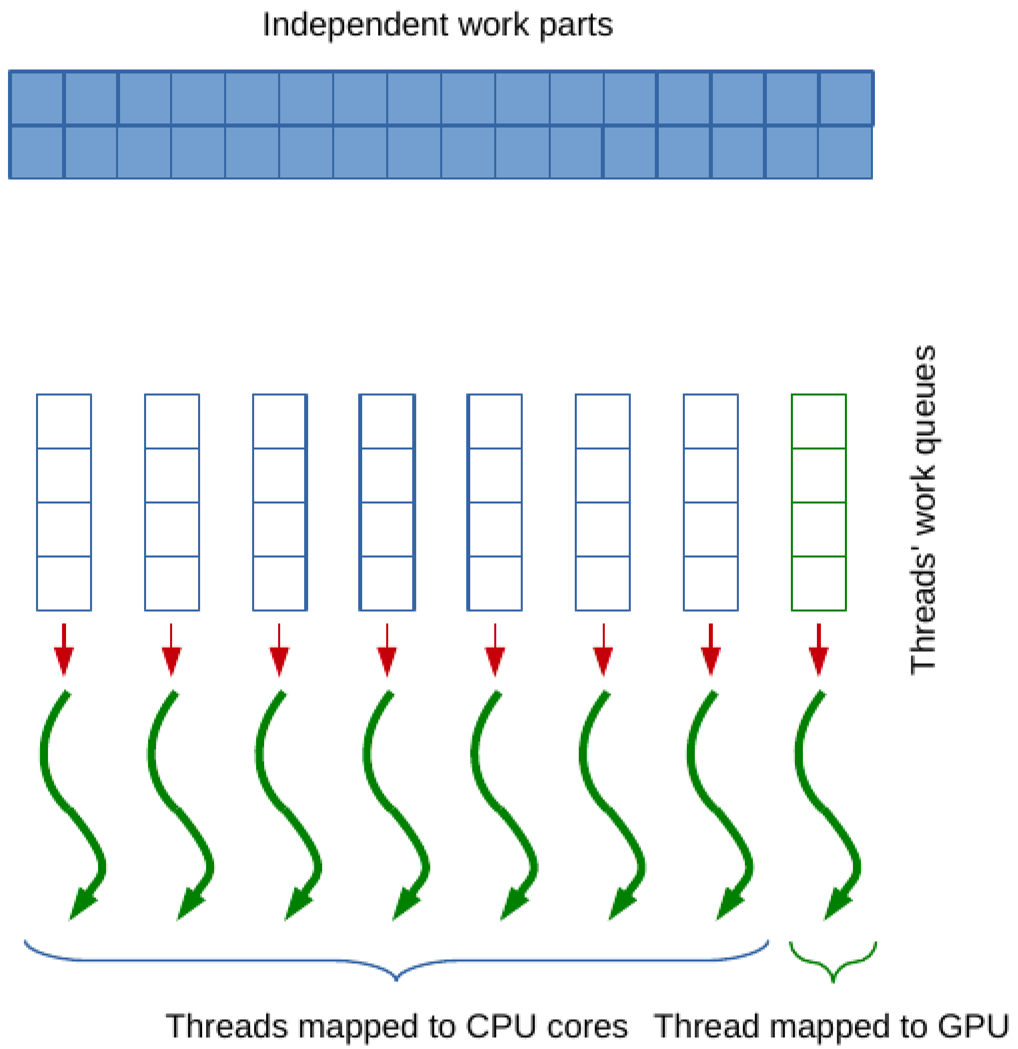

Time iteration step i
Solve for policy $\{p(g)\}_{g\in G}$, $G = \bigcup_{m=1}^{M} G_m$
MPI process 1
...
... MPI process M
Solve for $\{p(g)\}_{g\in G_1}$ given policy p from the previous iteration step
Solve for $\{p(g)\}_{g\in G_M}$ given policy p from the previous iteration step
TBB - CUDA/Thrust Kernel
GPU
Thread 1
Thread K
Merge $\{p(g)\}_{g\in G} = \bigcup_{m=1}^{M} \{p(g)\}_{g\in G_m}$
Proceed to step $i + 1$
Refinement of grid level L

With discrete states


Time iteration step *i*
MPI_COMM_WORLD splitted into N_S MPI_Groups of size M,...,T
MPI_Group of state z = 1
MPI_Group of state z = N_s
Solve for policy {p(z = 1,x)}_{x∈G} G = ∪_{m=1}^{M} G_m
Solve for policy {p(z = N_s, x)}_{x∈G} G = ∪_{m=1}^{T} G_m
MPI process 1
MPI process M
MPI process T
Solve for {p(z=1,x)}_{x∈G_1} given policy p_next = {p(1),...,p(N_s)} from the previous iteration step
TBB – CUDA Kernel
Thread 1
Thread K
GPU
Merge policy {p(z = 1,x)}_{x∈G} = ∪_{m=1}^{M} {p(z=1,x)}_{x∈G_M}
Merge policy {p(z=N_s,x)}_{x∈G} = ∪_{m=1}^{T} {p(z=N_s, x)}_{x∈G_T}
Refinement of grid level l = l + 1
MPI_Barrier(MPI_COMM_WORLD) p_next = ((p(1),...,p(N_S))
Proceed to iteration step *i+1*

Intel® Threading Building Blocks (TBB)

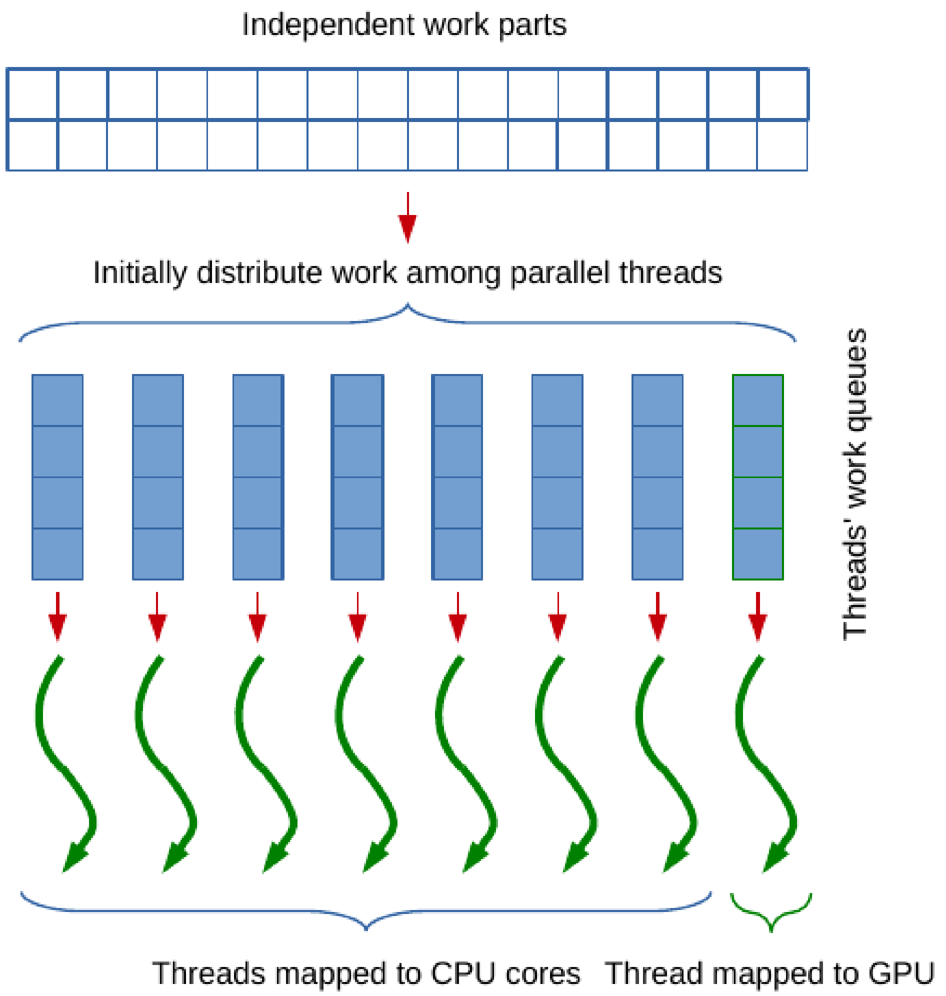
-TBB maps different threads, similar to OpenMP.



Intel® Threading Building Blocks (TBB)

-TBB maps different threads, similar to OpenMP.

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


Independent work parts
Initially distribute work among parallel threads
Threads' work queues
Threads mapped to CPU cores
Thread mapped to GPU

Intel® Threading Building Blocks (TBB)

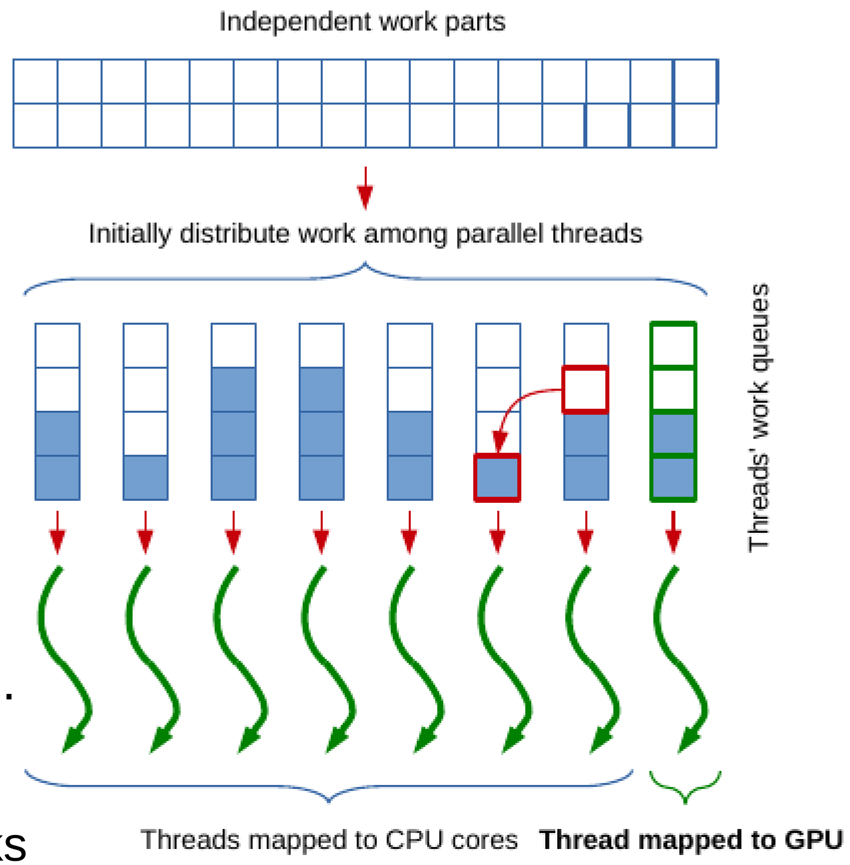
-TBB maps different threads, similar
 to OpenMP.

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

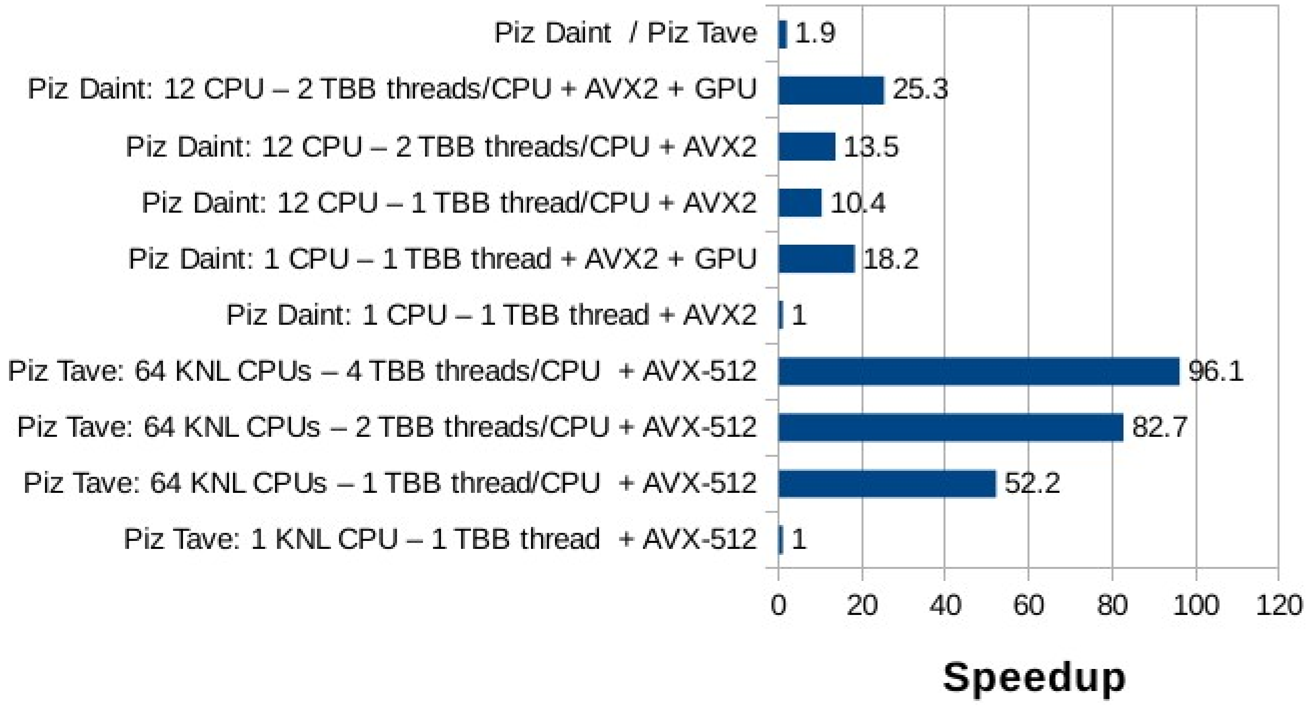
-However, different tasks may be
 processed faster or slower,
 due to differences between tasks and/or
 compute cores

-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.


Independent work parts
Initially distribute work among parallel threads
Threads' work queues
Threads mapped to CPU cores
Thread mapped to GPU

Strong scaling – 1 node



Strong scaling – intra-node

Scheidegger et al. (2018)

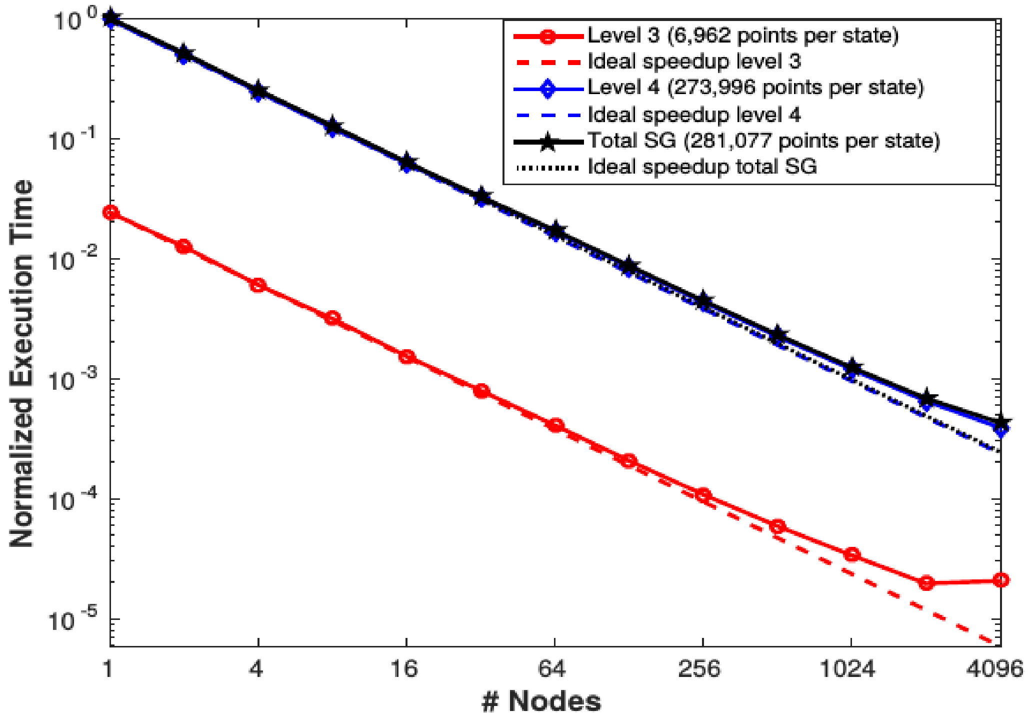


Figure 6: Strong scaling on Piz Daint for an OLG model using 4 levels of grid refinements, 16 discrete states, and $16 \cdot 281,077 = 4,497,232$ points and $265,336,688$ unknowns in total. "Total SG" shows the entire, normalized simulation time up to $4,096$ nodes. We also show normalized execution 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.

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

Time to soluton

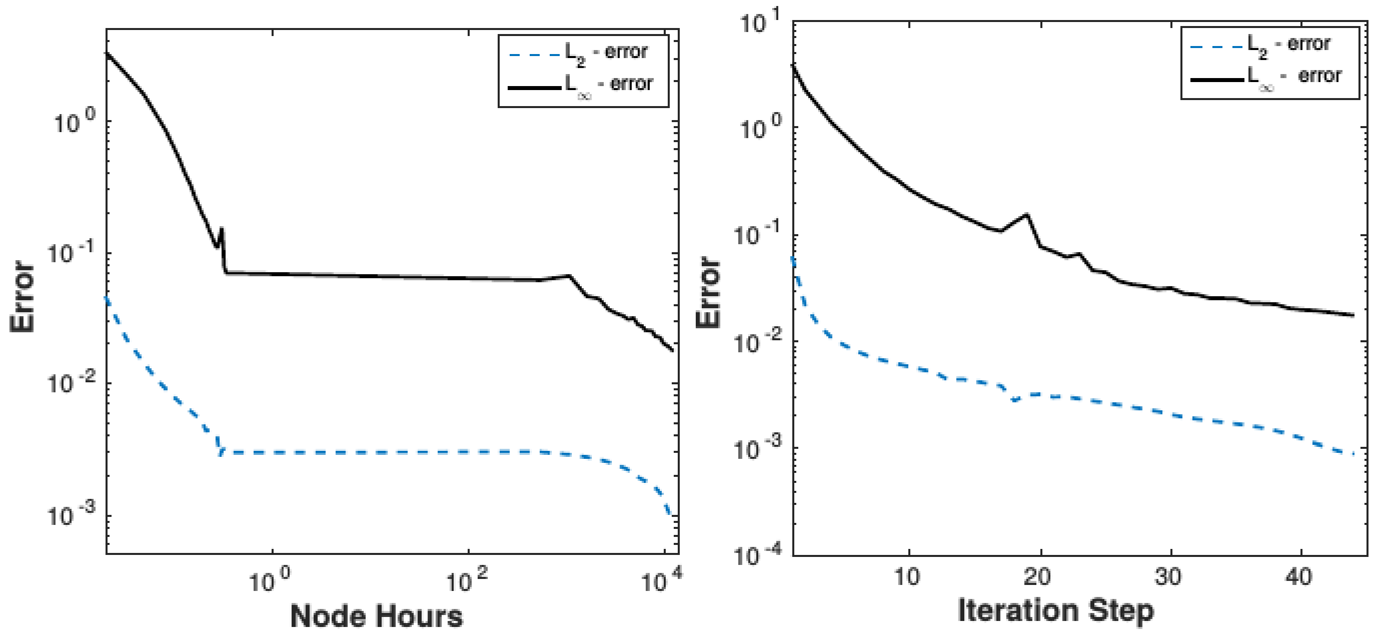


Figure 7: Comparison of the L_2 and L_∞−error for adaptive sparse grid solutions of the 59-dimensional OLG model as a function of compute time or iterations spent on Piz Daint.

Questions?

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