Hybrid parallel programming

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July 25th, 2019
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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
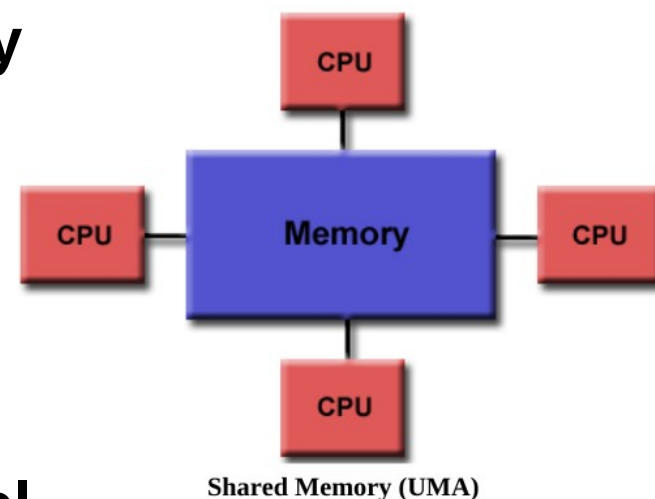
Putting things together:

   - Time Iteration, Adaptive Sparse Grids, HPC

Shared memory systems – OpenMP

- **Process can access same GLOBAL memory**

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

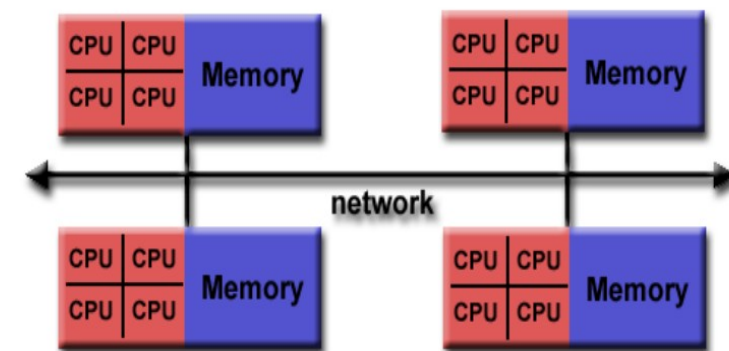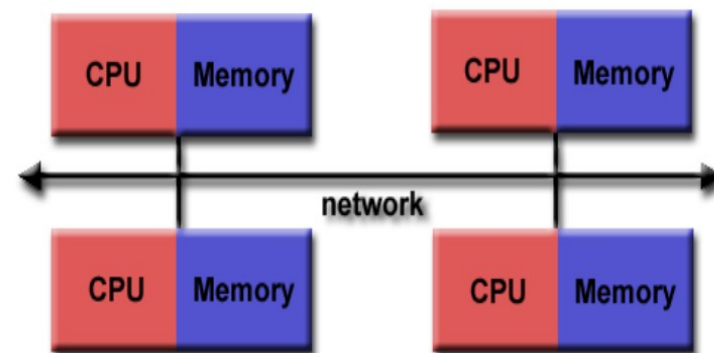Shared Memory (UMA)

- **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).
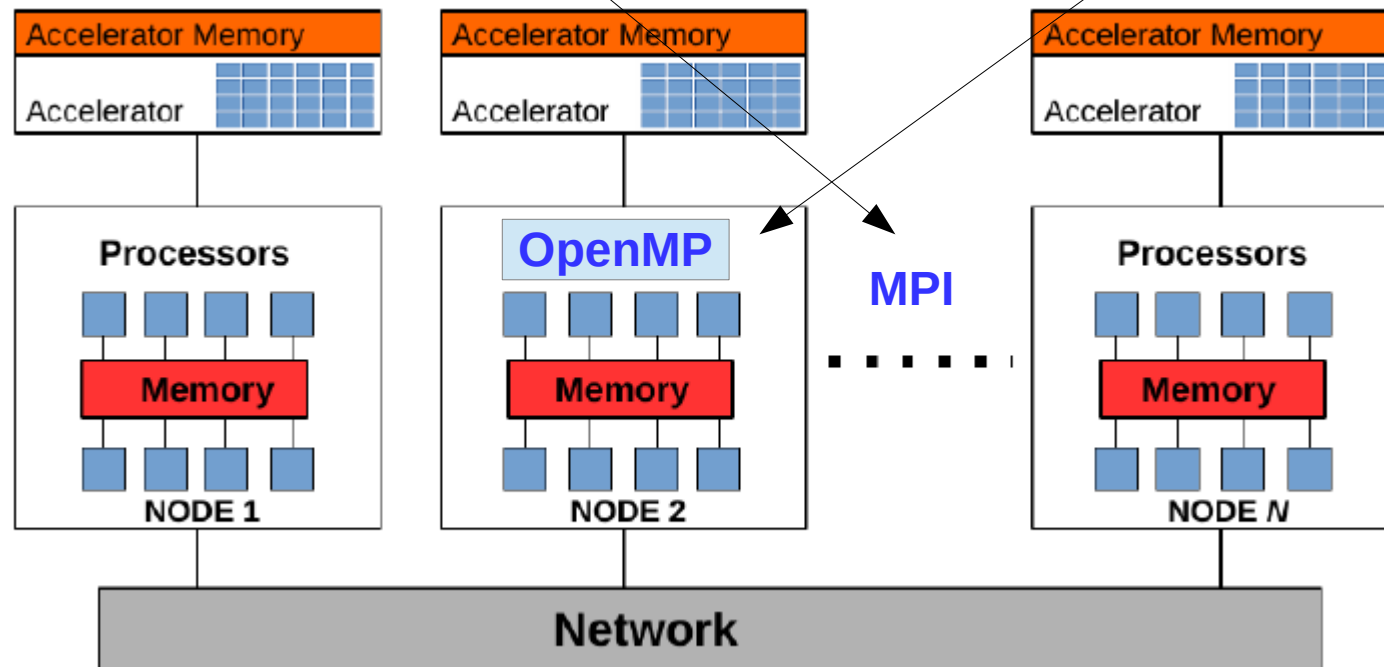

Shared Memory (NUMA)
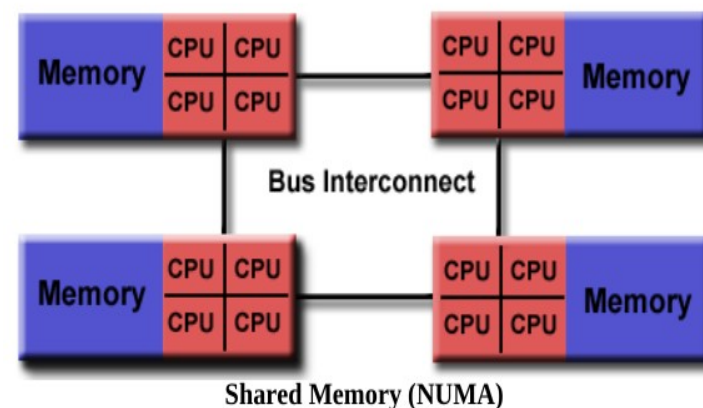
Distributed-memory parallel programming – MPI

- 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.
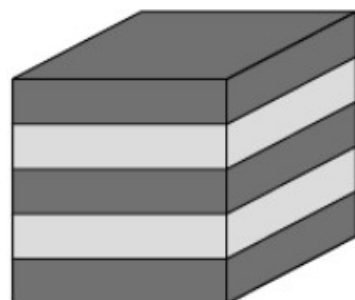
The hybrid MPI & OpenMP model

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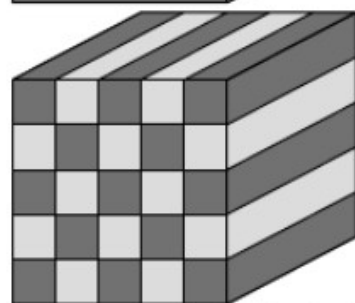
The hybrid MPI & OpenMP model has light-weight threads that share on-node memory.
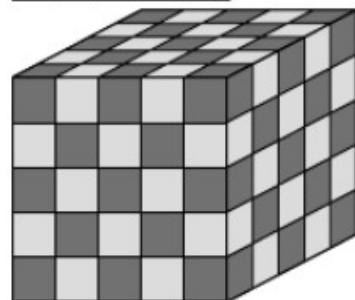
Domain decomposition

"Slabs"

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

"Poles"

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

"Cubes"

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

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"

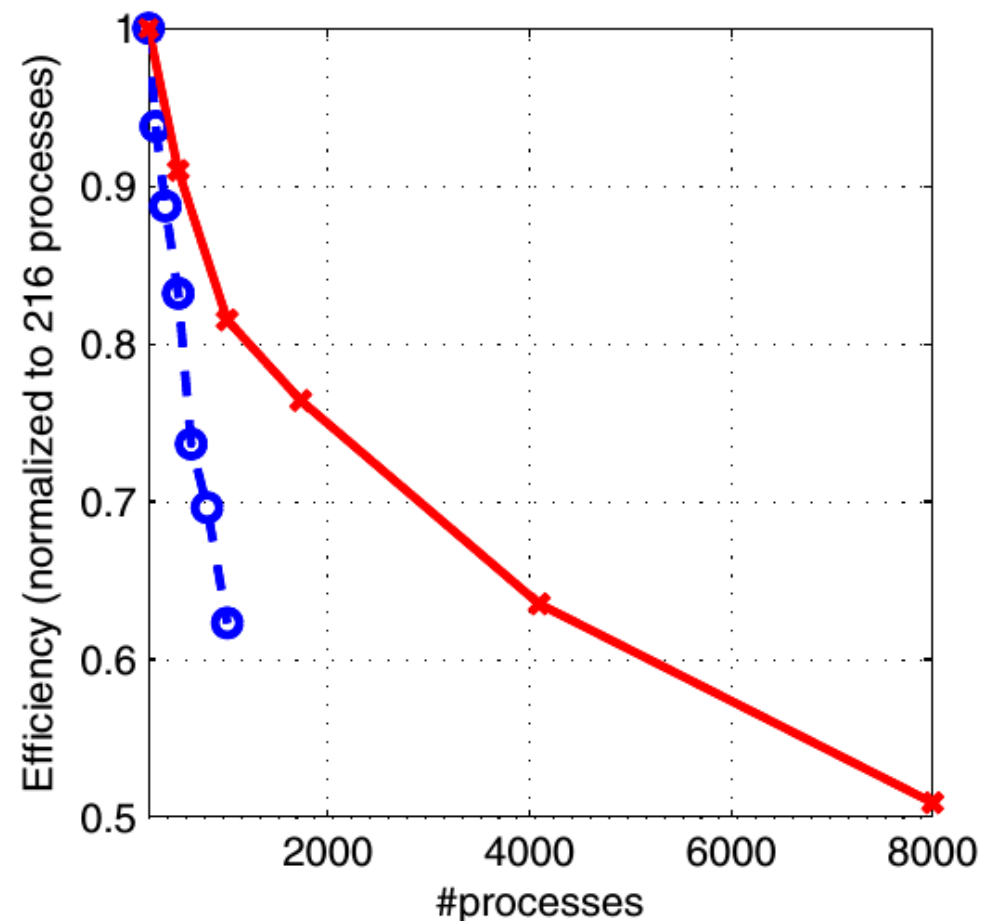See, e.g., Käppeli et al. (2011) http://iopscience.iop.org/article/10.1088/0067-0049/195/2/20/pdf

Hybrid parallelization:
→ Reduces the amount of memory consumption.
→ Reduces the amount of communication required.
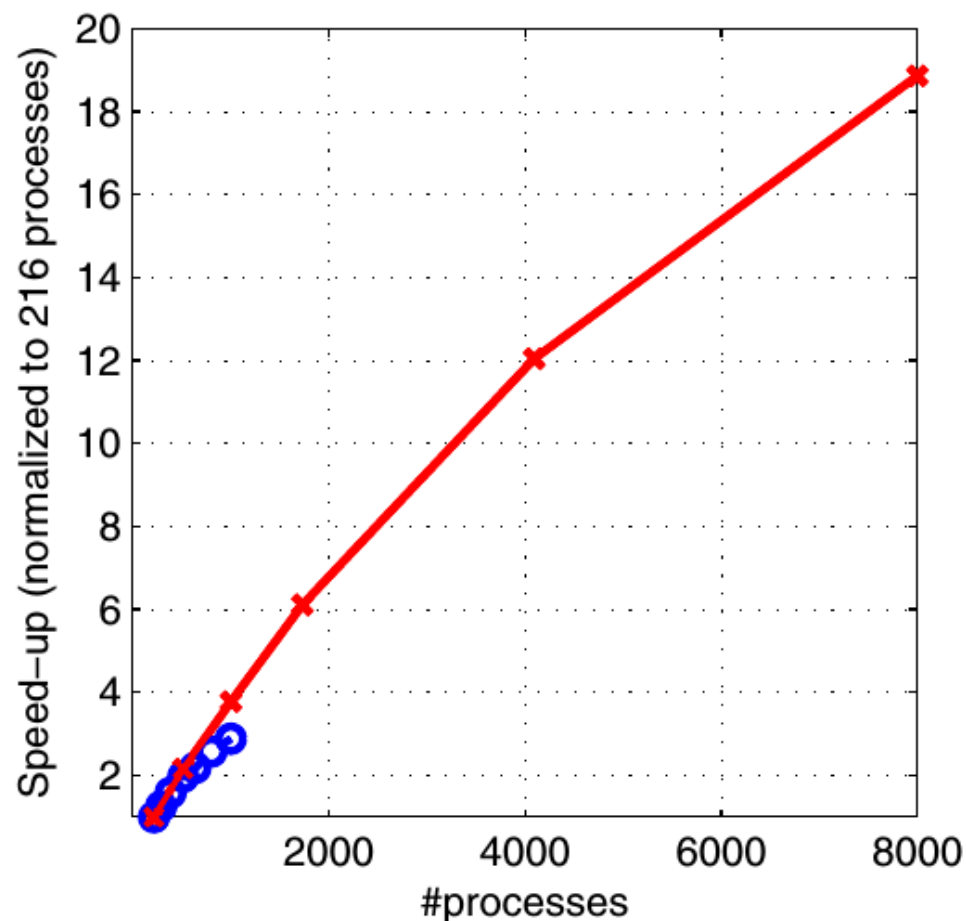
Hybrid parallelism with MPI and OpenMP

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)

Hybrid parallelism
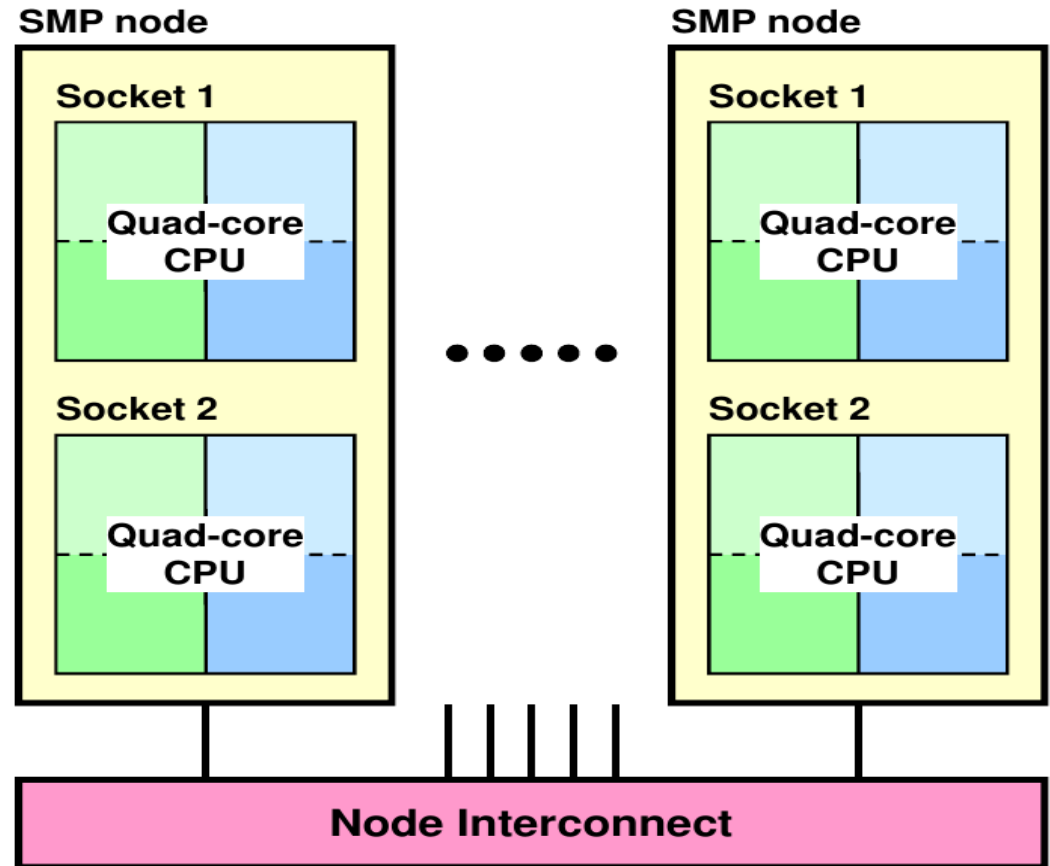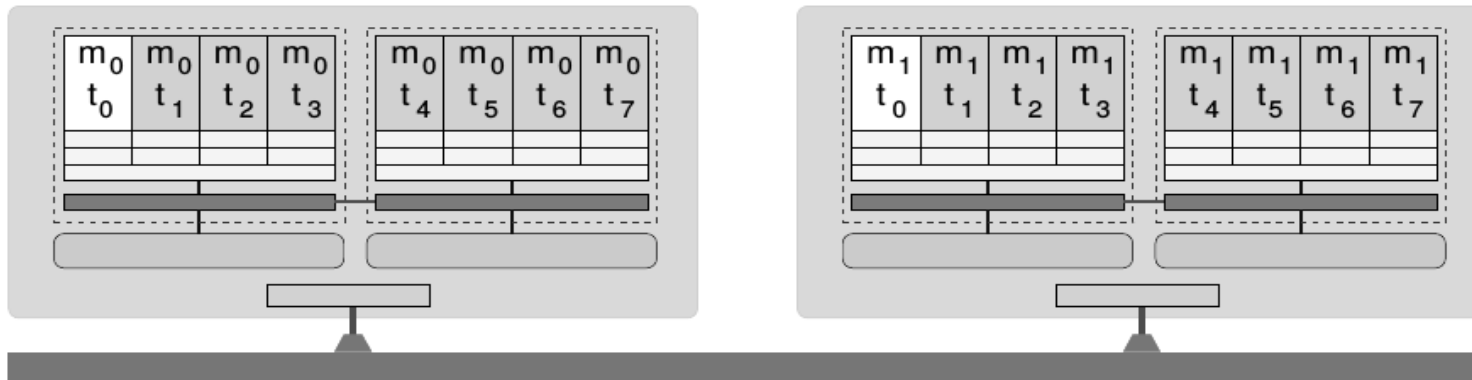
Mapping (2)

Figure 11.3: Mapping a single MPI process with eight threads to each node.
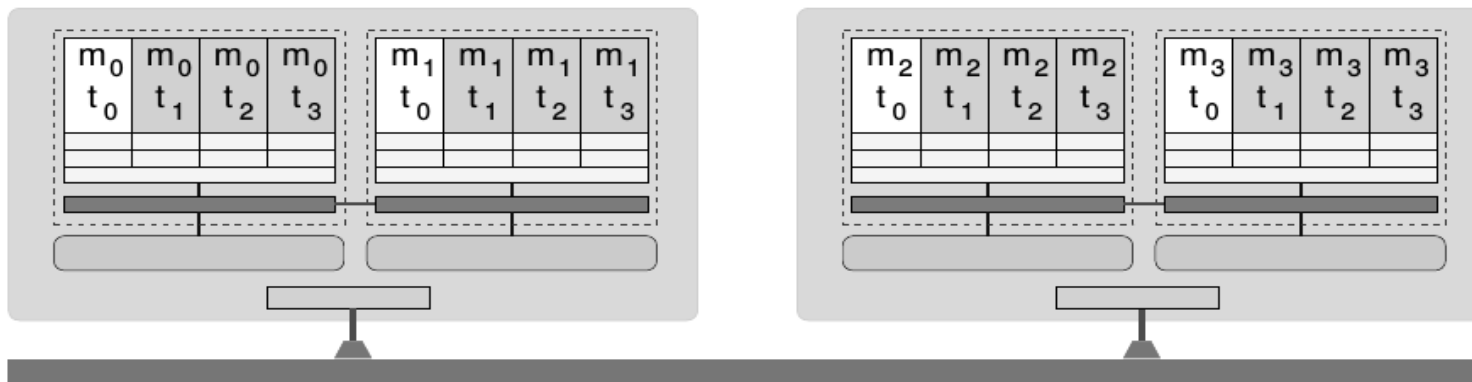
Figure 11.4: Mapping a single MPI process with four threads to each socket (L3 group or locality domain).

From Hager & Wellein (2011)
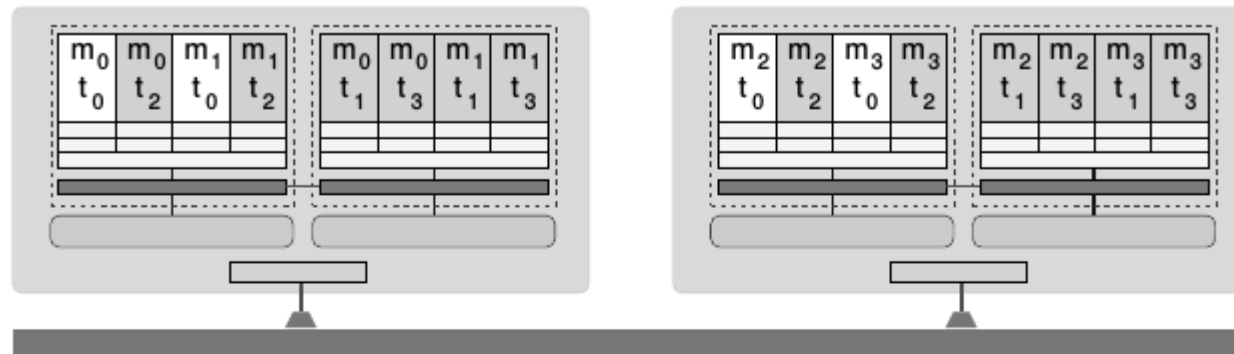
Mapping (3)

Figure 11.5: Mapping two MPI processes to each node and implementing a round-robin thread distribution.
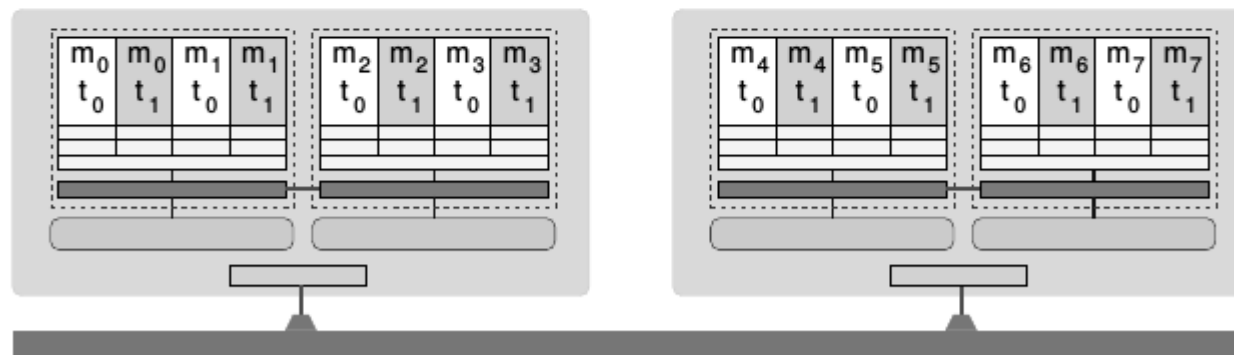
Figure 11.6: Mapping two MPI processes with two threads each to a single socket.

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
                                        C/C++

```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
#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();
```

21

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

```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
```

Node 1		Node 2	
Socket 1	Socket 2	Socket 1	Socket 2
Cores 0-7	Cores 8-15	Cores 0-7	Cores 8-15
Rank 0 0;1 / Rank 1 2;3 / Rank 2 4;5 / Rank 3 6;7	Rank 0 8;9 / Rank 1 10;11 / Rank 2 12;13 / Rank 3 14;15	Rank 4 0;1 / Rank 5 2;3 / Rank 6 4;5 / Rank 7 6;7	Rank 4 8;9 / Rank 5 10;11 / Rank 6 12;13 / Rank 7 14;15
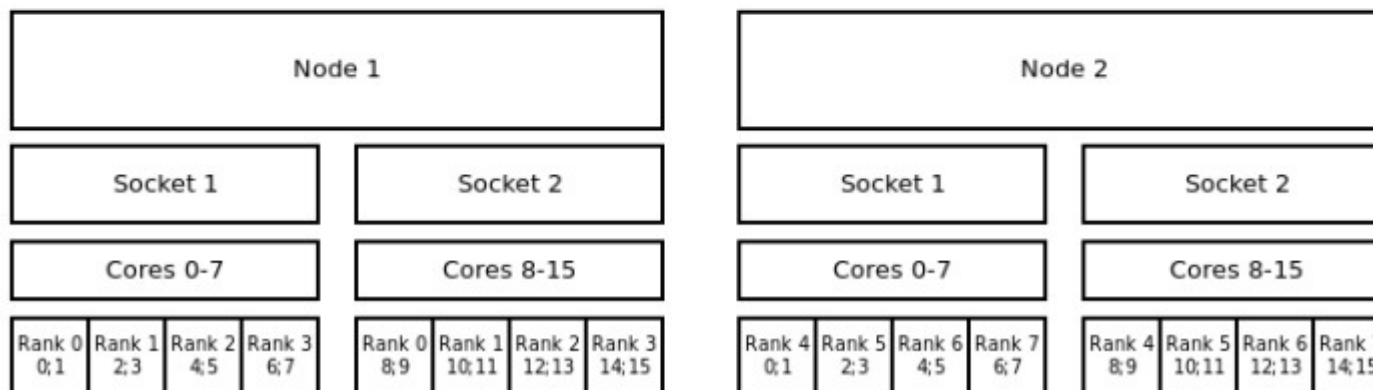
Example 2: Slurm on Midway

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

Hybrid parallelism

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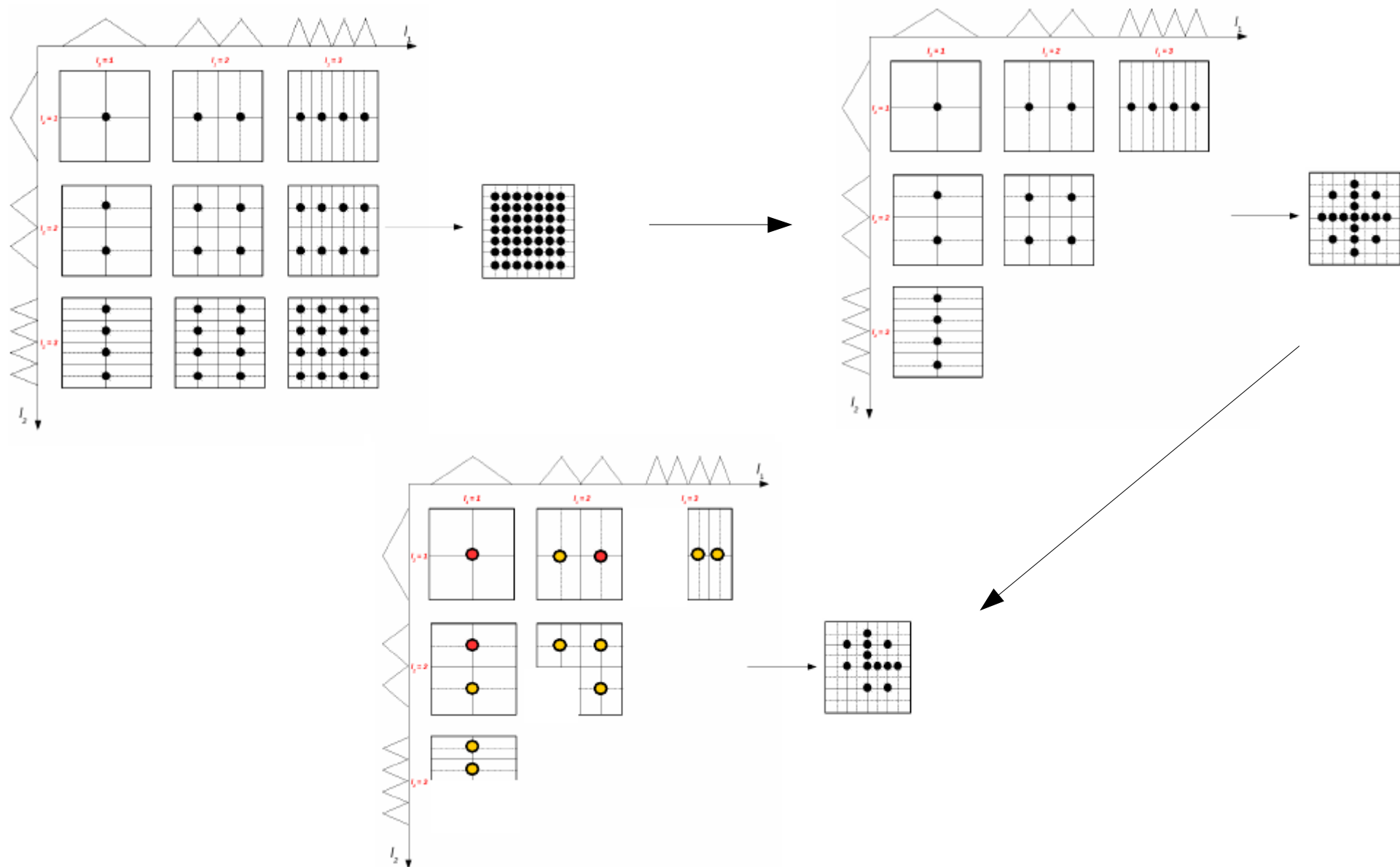
Putting things together: Time Iteration, Adaptive Sparse Grids, HPC

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 ϵ.

Result: The (approximate) equilibrium policy function $p = (p(1), \dots, p(N_s = 16))$.   Each state at each time period is independent

while $\eta > \bar{\eta}$ **do**

    Set $z = 1$.

    for $z \leq N_s$ **do**   For each state you split the comm_world in N_s groups

        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 each state I generate a sparse grid

            for $g(z) \in G(z) \setminus G_{old}(z)$ **do**   For each grid, all the grid points are independent, I can parallelize again

                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 $\{p(g(z))\}_{g(z) \in G_{old}(z)}$.   For each groups you split the number of points to different nodes, and for each node you split again the number of points for each threads

                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

Example:
- comm_world has 100 nodes
- you take 10 nodes for 10 states
- (each node has 10 CPUs)
- each node has 10 threads

        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 $\{p(g(z))\}_{g(z) \in G(z)}$.

If you have 1000 points for grid:
- 100 points to each node
- (10 points to each CPUs)
- 10 points to each thread

    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
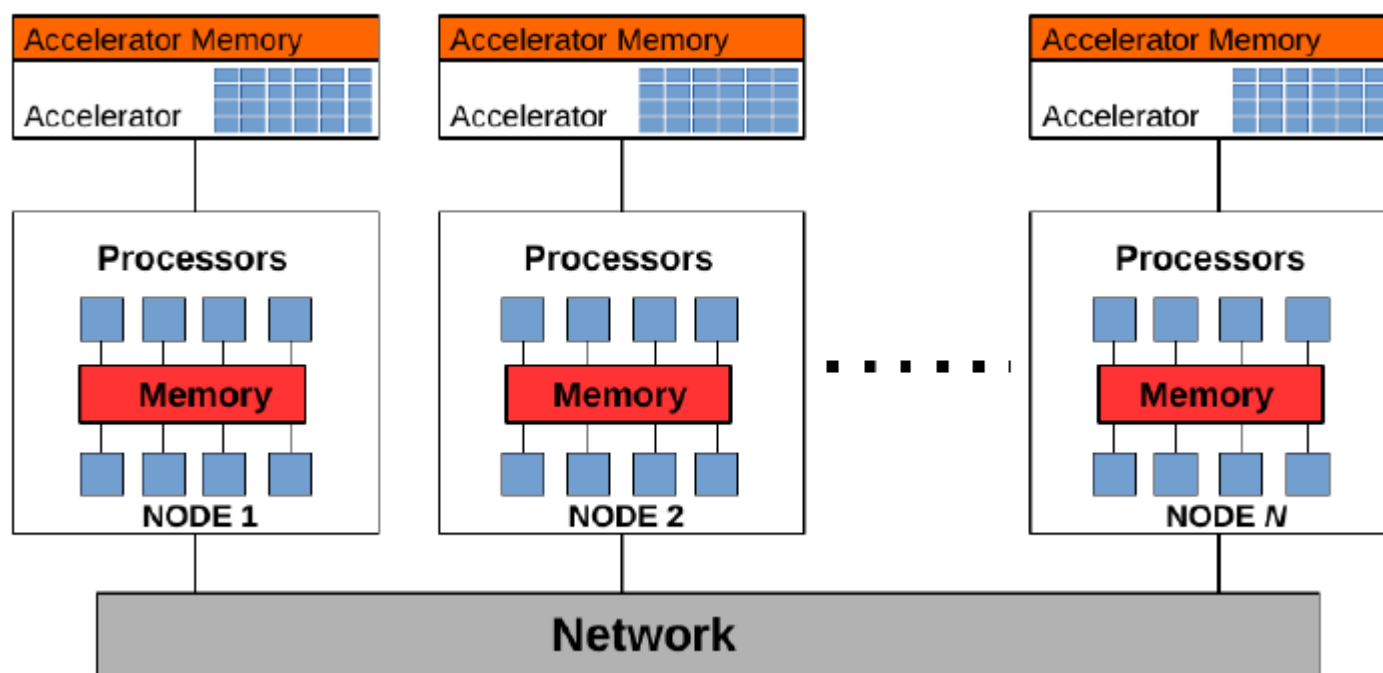
    error: $\eta = \max(\eta(1), \dots, \eta(N_s))$

end

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)
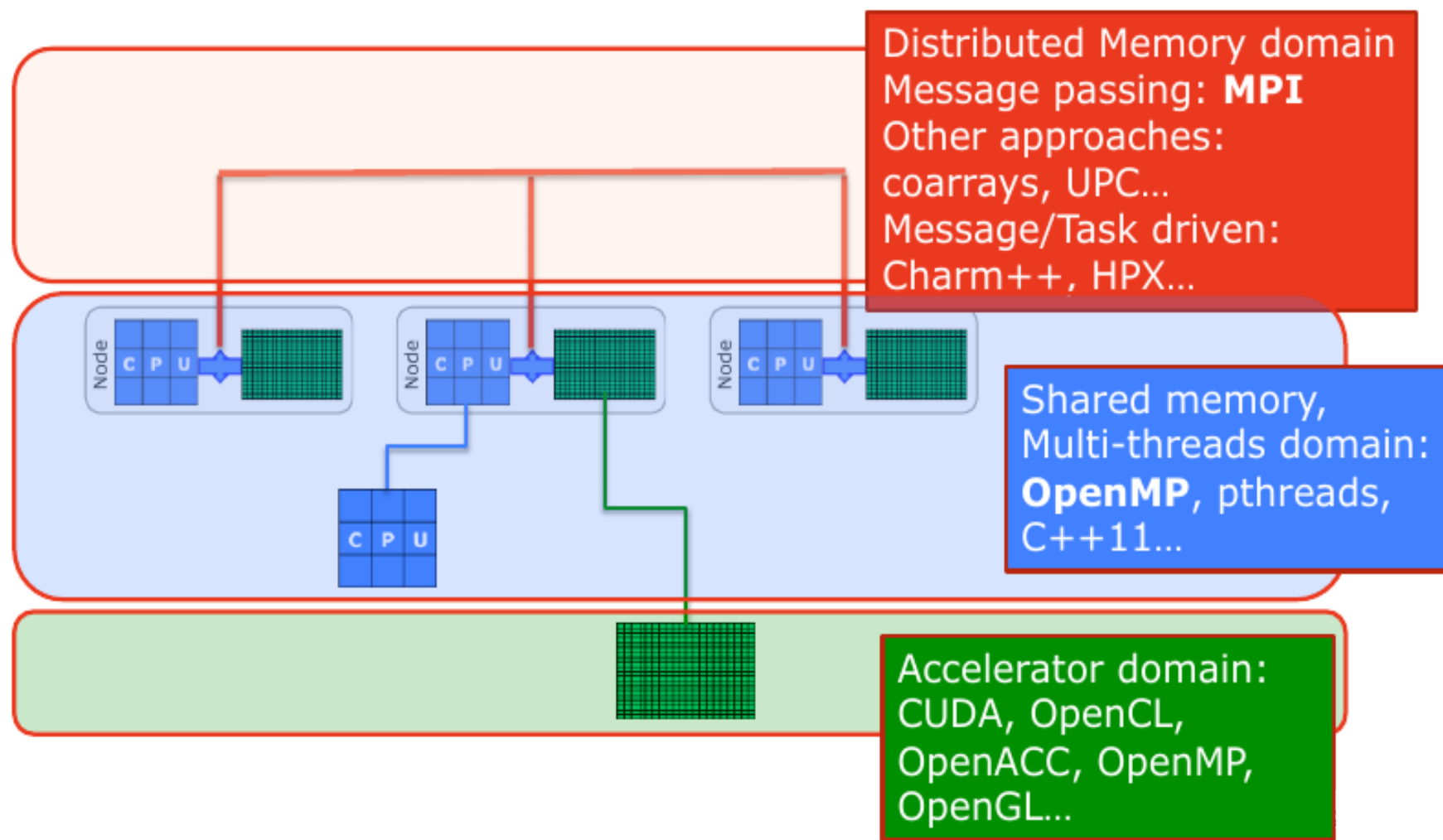
Parallel time iteration/DP algorithm

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

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

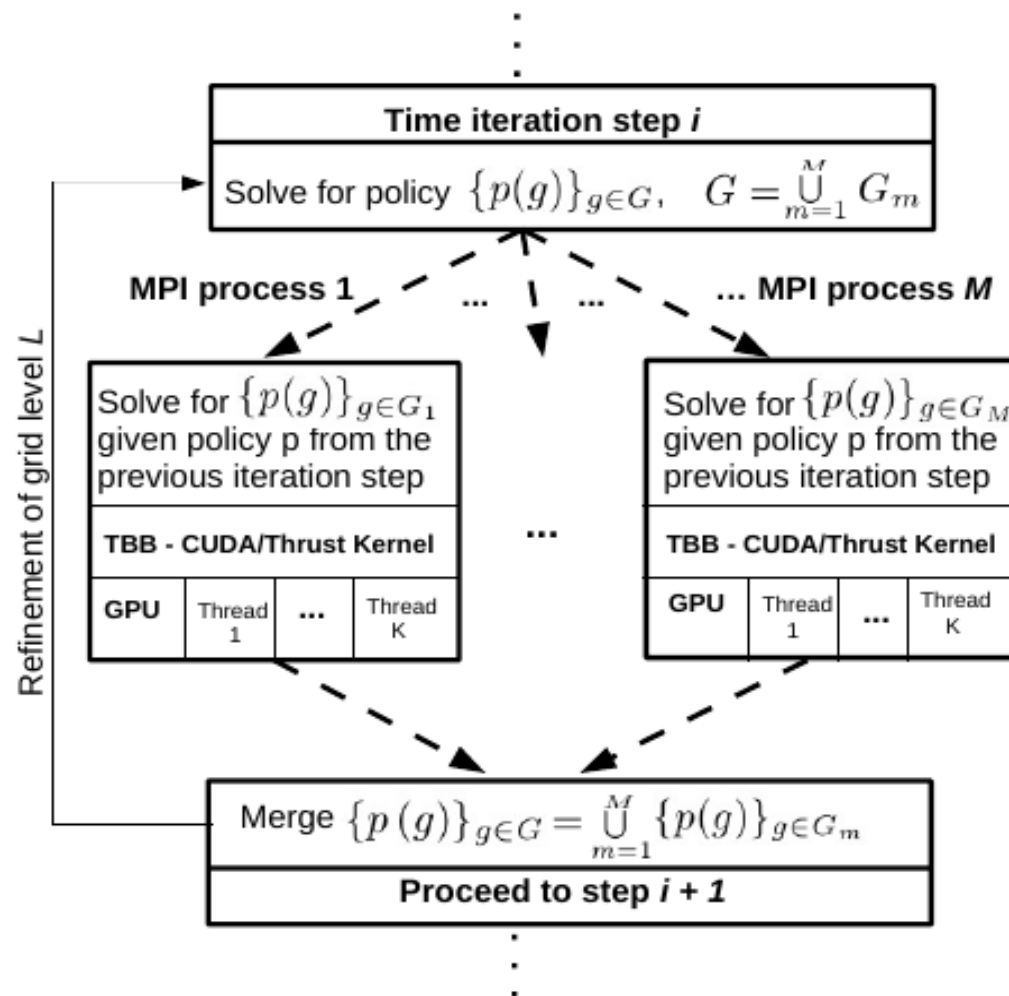-newly generated points are
 distributed via MPI

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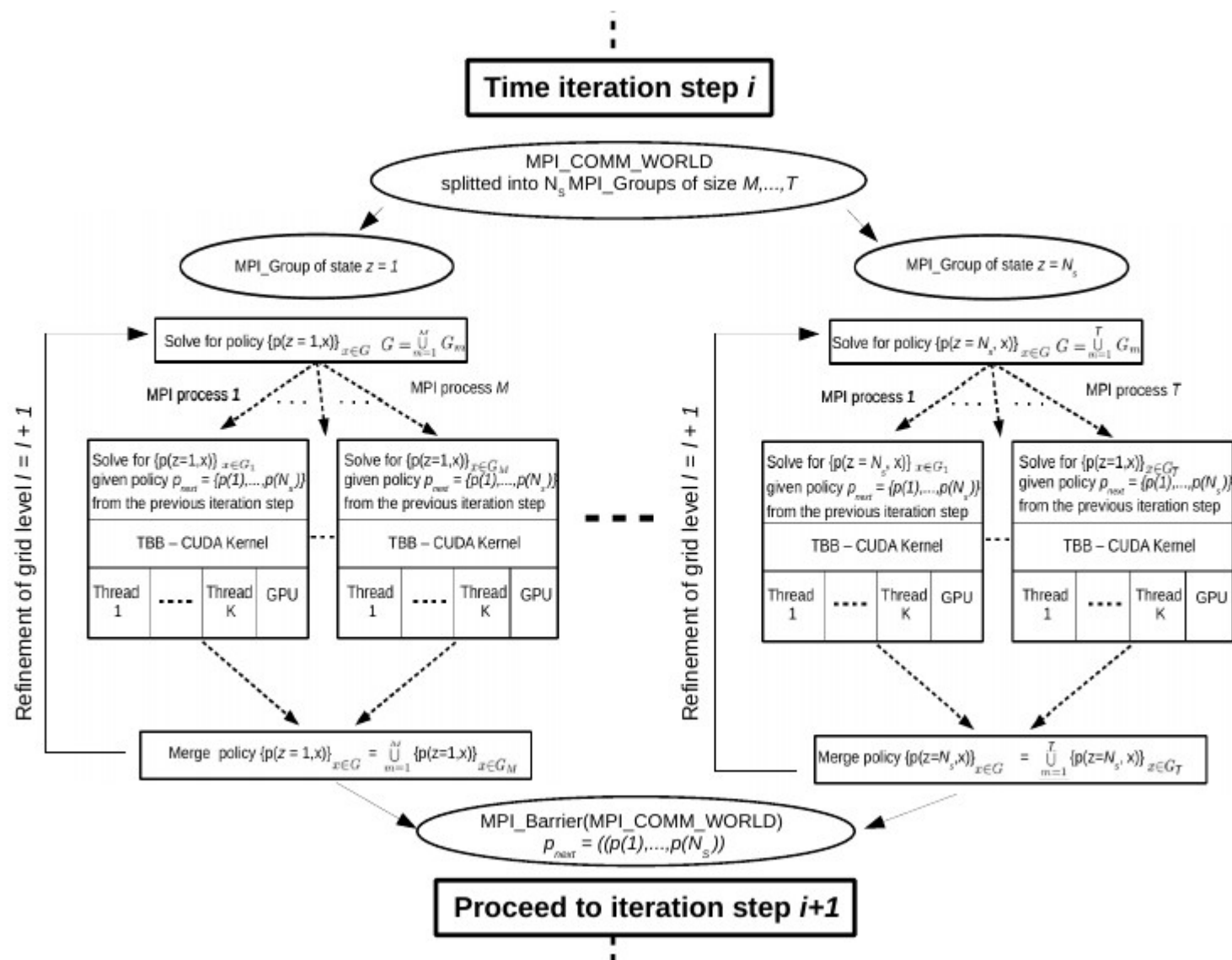(e.g. IPOPT (Waechter & Biegler (2006)).

In parallel: `messy' !

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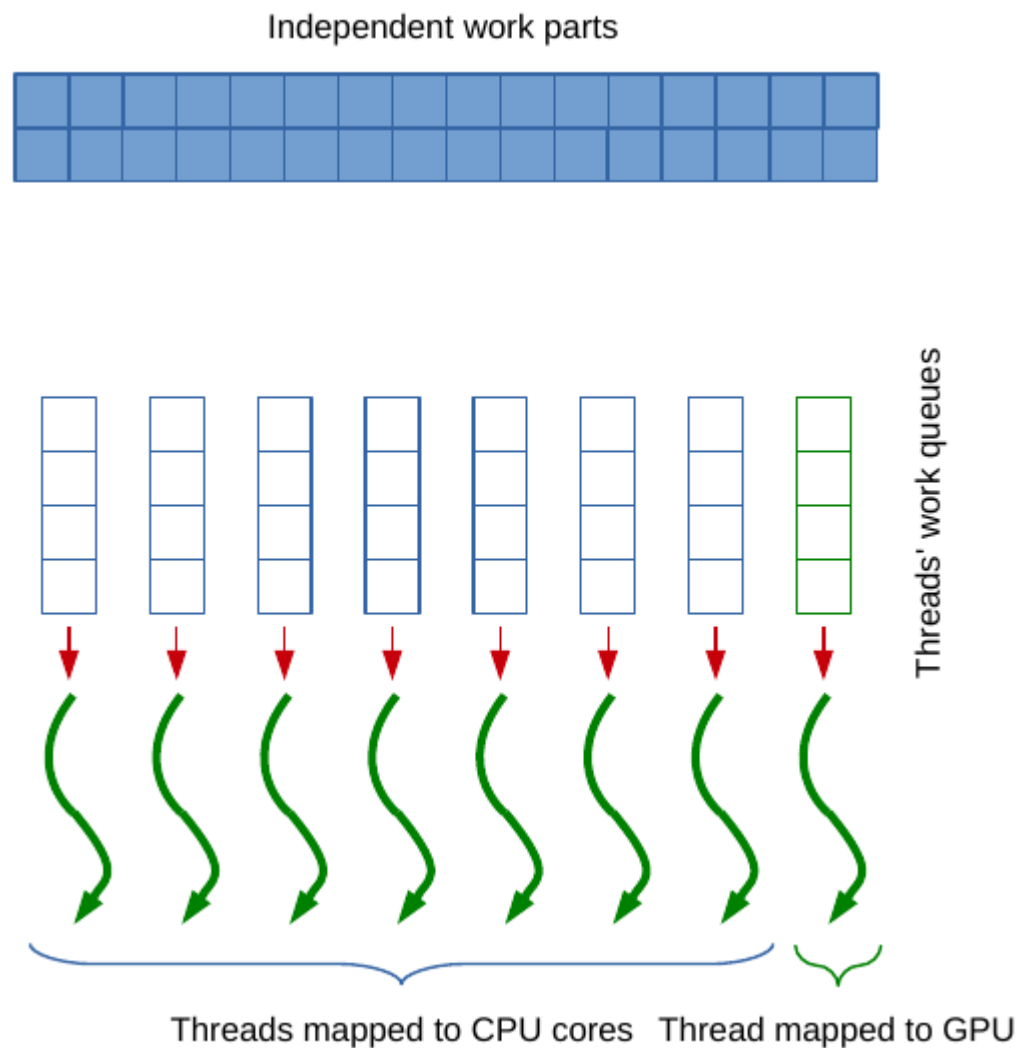→ **Now a lot better with TBB**

One single time-step

Time iteration step i
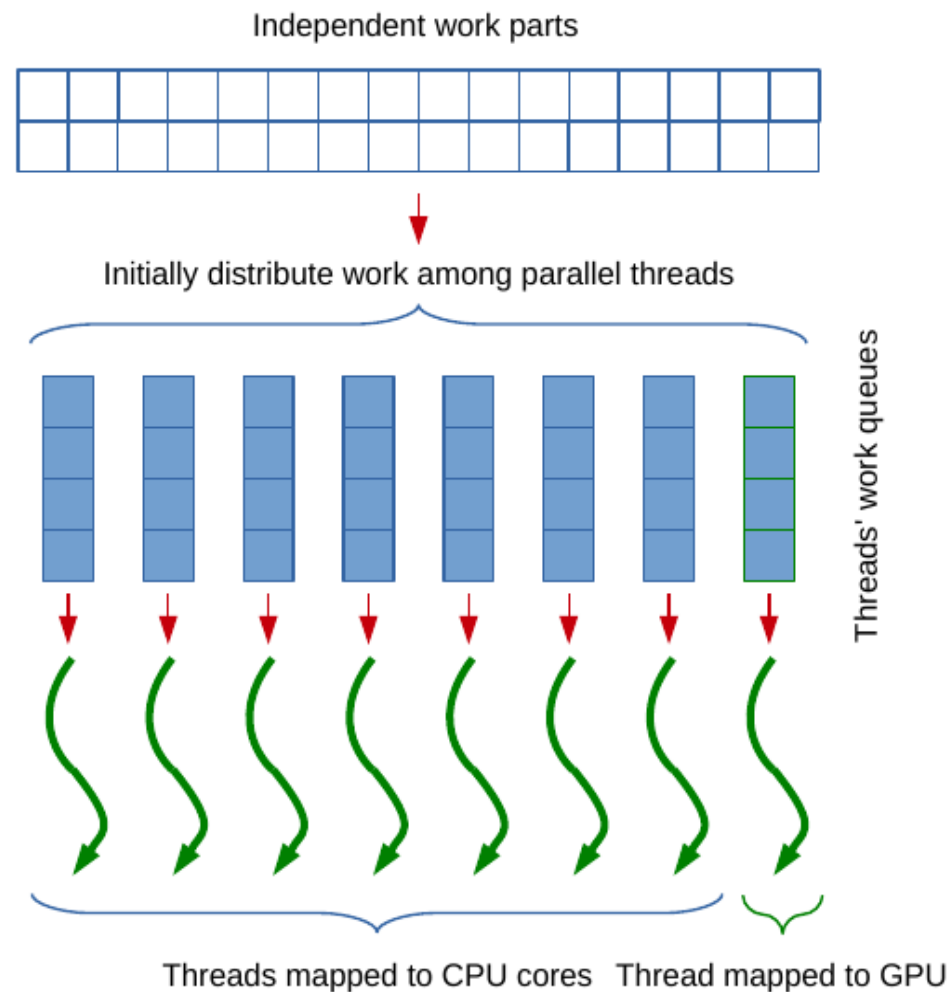
Solve for policy $\{p(g)\}_{g \in G}$, $G = \overset{M}{\underset{m=1}{\cup}} G_m$

Refinement of grid level L

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

TBB - CUDA/Thrust Kernel

GPU | Thread 1 | ... | Thread K

Merge $\{p(g)\}_{g \in G} = \overset{M}{\underset{m=1}{\cup}} \{p(g)\}_{g \in G_m}$

Proceed to step $i + 1$

With discrete states

Intel® Threading Building Blocks (TBB)

-TBB maps different threads, similar
 to OpenMP.

Independent work parts

Threads' work queues
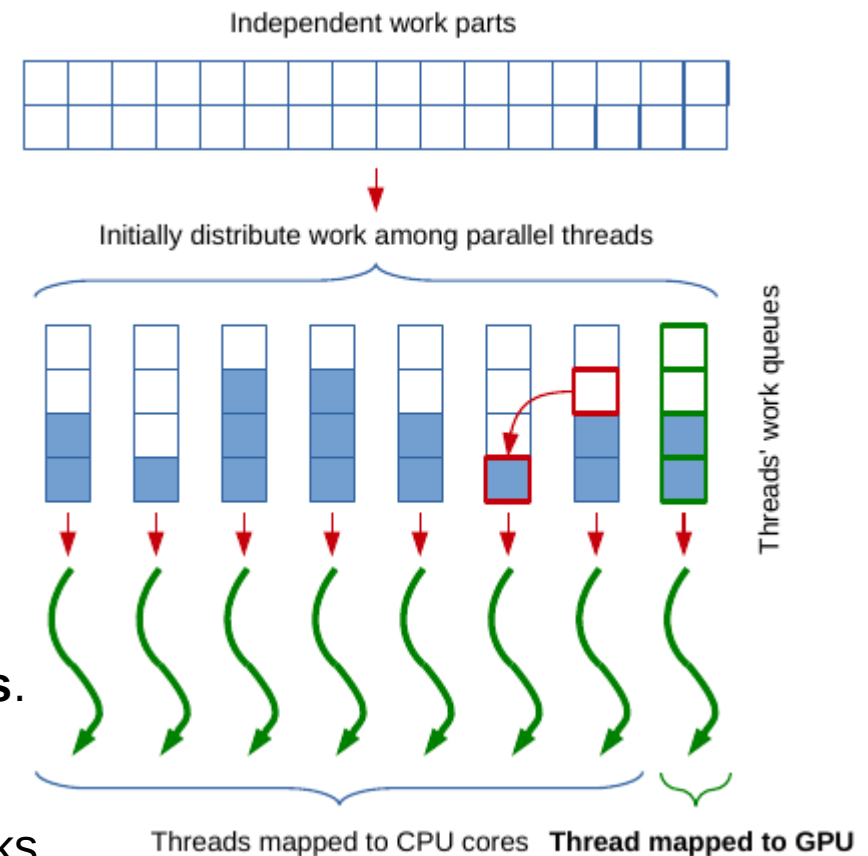
Threads mapped to CPU cores   Thread mapped to GPU

Intel® Threading Building Blocks (TBB)

-TBB maps different threads, similar to OpenMP.

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

Independent work parts

Initially distribute work among parallel threads

Threads' work queues
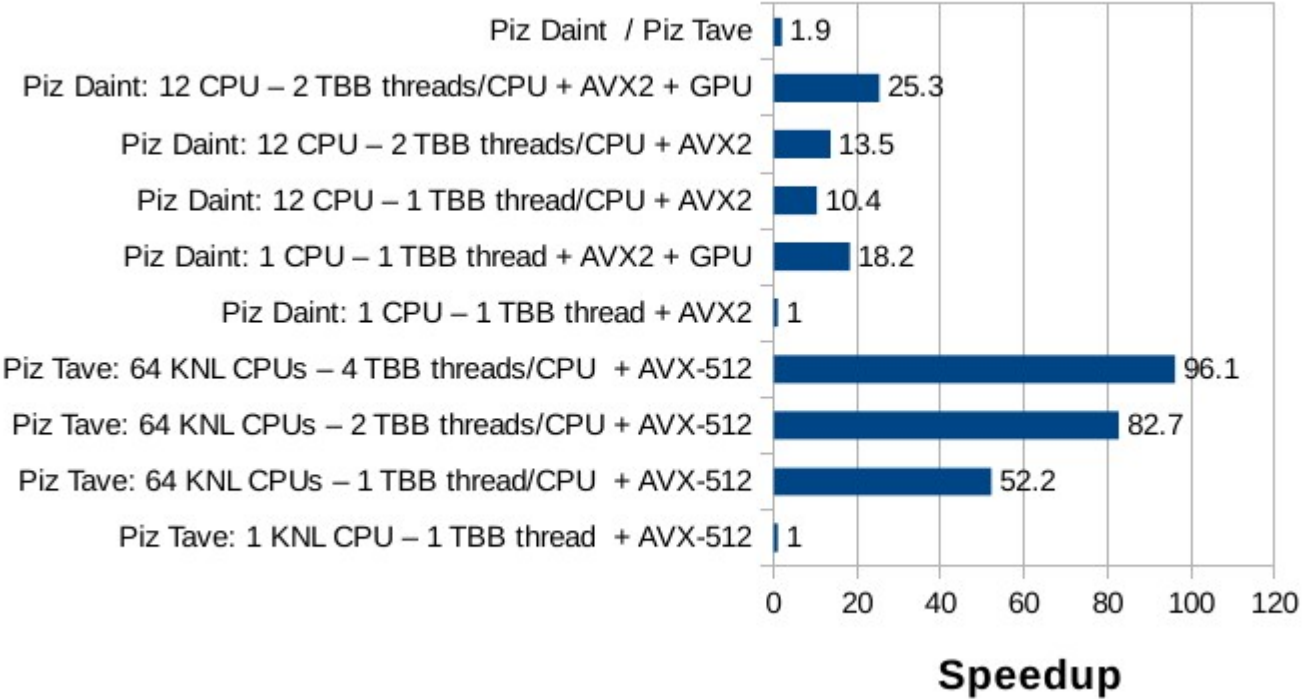
Threads mapped to CPU cores   Thread mapped to GPU

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**
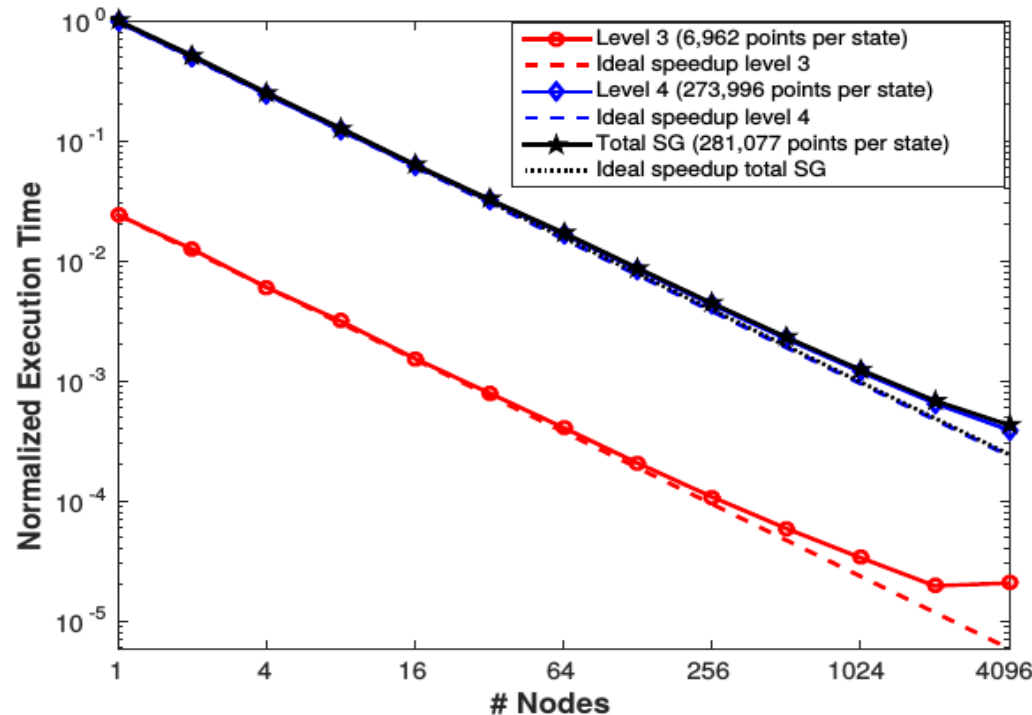 → **CPU** cores and **GPU** process interpolation tasks
 together.

Independent work parts

Initially distribute work among parallel threads

Threads' work queues

Threads mapped to CPU cores   **Thread mapped to GPU**

Sparse Grids & HPC

Strong scaling – 1 node

Strong scaling – intra-node

Scheidegger et al. (2018)

- 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.
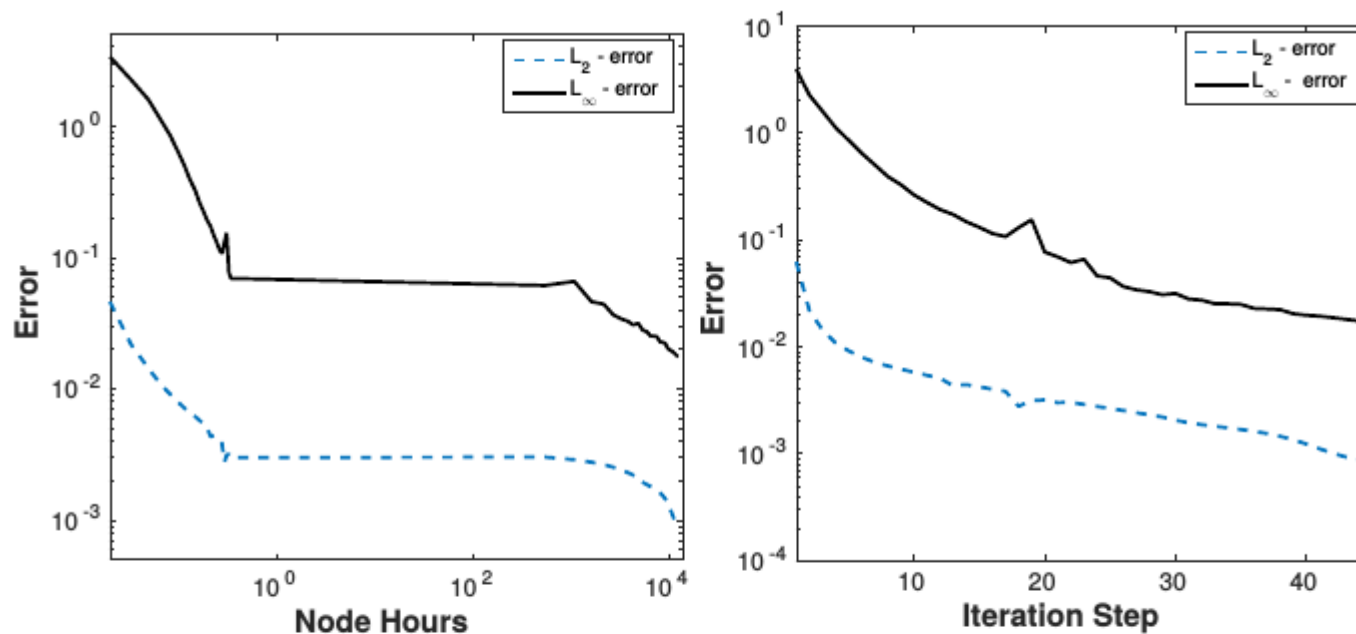
Time to soluton

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?

?