Hybrid MPI and OpenMP Parallel Programming

MPI + OpenMP and other models on clusters of SMP nodes

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Invited Talk in the Lecture

"Cluster-Computing"

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Outline slide number Introduction / Motivation Programming models on clusters of SMP nodes Mismatch Problems 21 - Topology problem 23 - Unnecessary intra-node communication 24 - Inter-node bandwidth problem 25 Sleeping threads and saturation problem Additional OpenMP overhead 37 - Overlapping communication and computation - Communication overhead with DSM No silver bullet Thread-safety quality of MPI libraries Summary 65 Appendix Hybrid Parallel Programming © Rolf Rabenseifner Slide 2 / 70 Höchstleistungsrechenzentrum Stuttgart H L R S



- Efficient programming of clusters of SMP nodes SMP nodes:
 - · Dual/multi core CPUs
 - · Multi CPU shared memory
 - Multi CPU ccNUMA
 - · Any mixture with shared memory programming model
- Hardware range
 - · mini-cluster with dual-core CPUs

 - · large constellations with large SMP nodes
- Hybrid MPI/OpenMP programming seems natural
 - · MPI between the nodes
 - · OpenMP inside of each SMP node
- Often hybrid programming slower than pure MPI
 - · Examples, Reasons, ...



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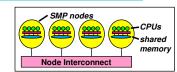




shared

memory

Motivation



- Using the communication bandwidth of the hardware optimal usage
- Minimizing synchronization = idle time

of the hardware

Appropriate parallel programming models / Pros & Cons



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But results may surprise!

- Example code HYDRA
- Domain-decomposed hydrodynamics
 - (almost) independent mesh domains with ghost cells on boundaries
 - ghost cells communicate boundary information ~40-50 times per cycle
- · Parallelism model: single level
 - MPI divides domains among compute nodes
 - OpenMP further subdivides domains among processors
 - domain size set for cache efficiency
 - · minimizes memory usage, maximizes efficiency
 - scales to very large problem sizes (>10⁷ zones, >10³ domains)
- Results:
 - MPI (256 proc.) ~20% faster than MPI / OpenMP (64 nodes x 4 proc./node)
 - domain-domain communication not threaded,
 i.e., MPI communication is done only by main thread
 - accounts for ~10% speed difference, remainder in thread overhead

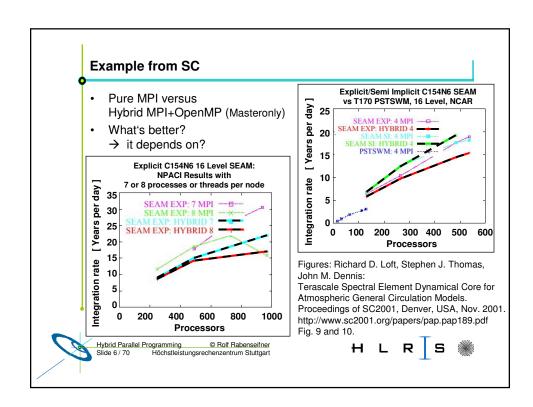




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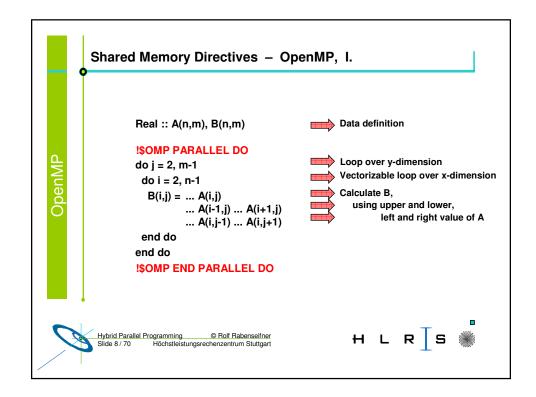


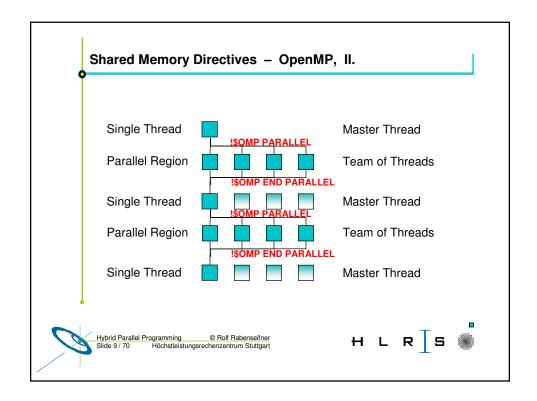


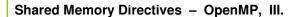
- Introduction / Motivation
- Programming models on clusters of SMP nodes
- Mismatch Problems
- Thread-safety quality of MPI libraries
- Summary





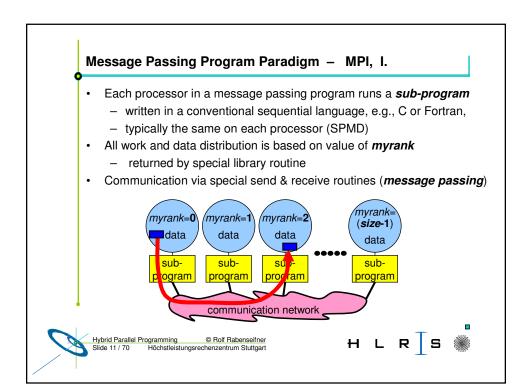


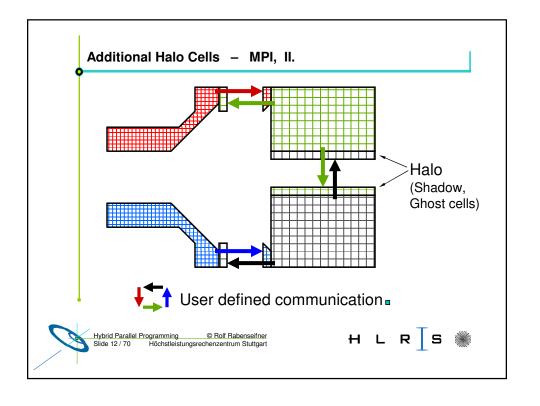




- OpenMP
 - standardized shared memory parallelism
 - thread-based
 - the user has to specify the work distribution explicitly with directives
 - no data distribution, no communication
 - mainly loops can be parallelized
 - compiler translates OpenMP directives into thread-handling
 - standardized since 1997
- · Automatic SMP-Parallelization
 - e.g., Compas (Hitachi), Autotasking (NEC)
 - thread based shared memory parallelism
 - with directives (similar programming model as with OpenMP)
 - supports automatic parallelization of loops
 - similar to automatic vectorization







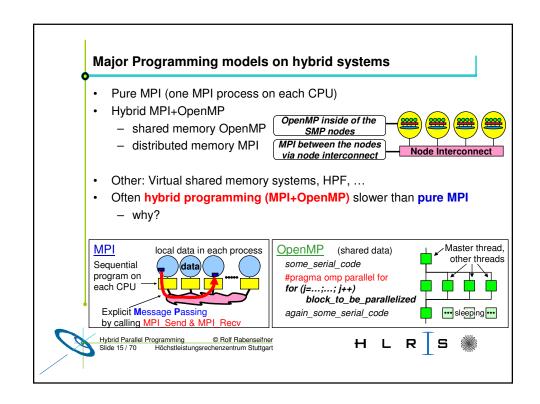
Message Passing - MPI, III. Call MPI Comm size(MPI COMM WORLD, size, ierror) Call MPI_Comm_rank(MPI_COMM_WORLD, myrank, ierror) m1 = (m+size-1)/size; ja=1+m1*myrank; je=max(m1*(myrank+1), m) jax=ja-1; jex=je+1 // extended boundary with halo Data definition Real :: A(n, jax:jex), B(n, jax:jex) do j = max(2,ja), min(m-1,je)Loop over y-dimension do i = 2, n-1 Vectorizable loop over x-dimension B(i,j) = ... A(i,j)Calculate B. ... A(i-1,j) ... A(i+1,j) using upper and lower, ... A(i,j-1) ... A(i,j+1) left and right value of A end do end do Call MPI_Send(......) !- sending the boundary data to the neighbors Call MPI_Recv(......) !- receiving from the neighbors, ! storing into the halo cells Hybrid Parallel Programming © Rolf Rabenseifner Slide 13 / 70 Höchstleistungsrechenzentrum Stuttgart H L R S

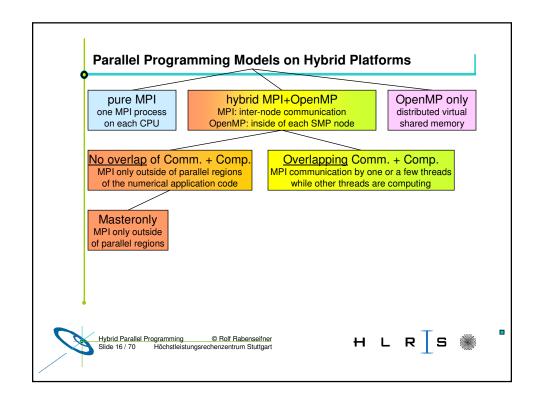
Summary — MPI, IV.

- MPI (Message Passing Interface)
 - standardized distributed memory parallelism with message passing
 - process-based
 - the user has to specify the <u>work distribution</u> & <u>data distribution</u>
 all <u>communication</u>
 - synchronization implicit by completion of communication
 - the application processes are calling MPI library-routines
 - compiler generates normal sequential code
 - typically domain decomposition is used
 - communication across domain boundaries
 - standardized
 MPI-1: Version 1.0 (1994), 1.1 (1995), 1.2 (1997)
 MPI-2: since 1997









Pure MPI

pure MPI one MPI process on each CPU

Advantages

- No modifications on existing MPI codes
- MPI library need not to support multiple threads

Major problems

- Does MPI library uses internally different protocols?
 - · Shared memory inside of the SMP nodes
 - · Network communication between the nodes
- Does application topology fit on hardware topology?
- Unnecessary MPI-communication inside of SMP nodes!



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Hybrid Masteronly

Masteronly MPI only outside of parallel regions

Advantages

- No message passing inside of the SMP nodes
- No topology problem

for (iteration)

#pragma omp parallel numerical code *end omp parallel */

on master thread only */ MPI_Send (original data to halo areas in other SMP nodes) MPI_Recv (halo data from the neighbors) } /*end for loop

Major Problems

- MPI-lib must support at least MPI_THREAD_FUNNELED
- Which inter-node bandwidth?
- All other threads are sleeping while master thread communicates!



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Overlapping Communication and Computation

MPI communication by one or a few threads while other threads are computing

```
if (my_thread_rank < ...) {
  MPI Send/Recv....
   i.e., communicate all halo data
} else {
  Execute those parts of the application
   that do not need halo data
   (on non-communicating threads)
Execute those parts of the application
 that need halo data
 (on all threads)
```



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Pure OpenMP (on the cluster)

OpenMP only distributed virtual shared memory

- Distributed shared virtual memory system needed
- Must support clusters of SMP nodes
- e.g., Intel® Cluster OpenMP
 - Shared memory parallel inside of SMP nodes
 - Communication of modified parts of pages at OpenMP flush (part of each OpenMP barrier)

i.e., the OpenMP memory and parallelization model is prepared for clusters!









Outline

- Introduction / Motivation
- Programming models on clusters of SMP nodes
- **Mismatch Problems**
- Thread-safety quality of MPI libraries
- Summary





[with pure MPI]

Mismatch Problems

Topology problem

Unnecessary intra-node communication [with pure MPI]

Inter-node bandwidth problem [with hybrid MPI+OpenMP]

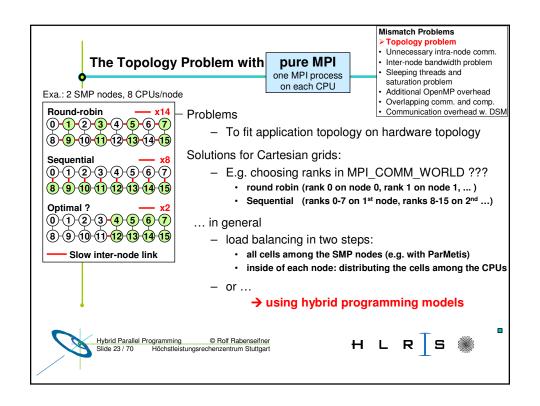
Sleeping threads and [with masteronly] saturation problem [with pure MPI]

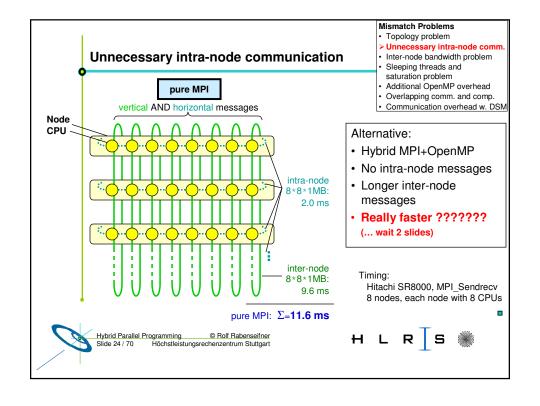
Additional OpenMP overhead [with hybrid MPI+OpenMP]

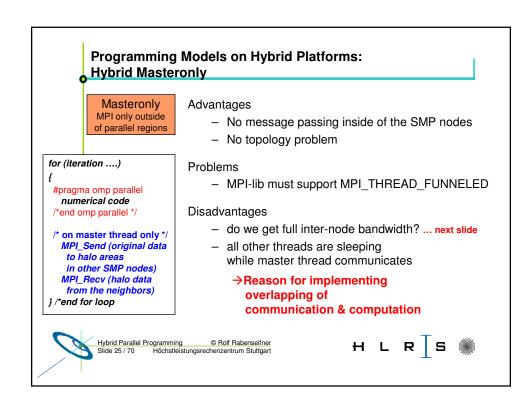
- Thread startup / join
- Cache flush (data source thread communicating thread sync. → flush)
- Overlapping communication and computation [with hybrid MPI+OpenMP]
 - → separation of local or halo-based code an application problem
 - a programming problem → thread-ranks-based vs. OpenMP work-sharing
 - a load balancing problem, if only some threads communicate / compute
- Communication overhead with DSM [with pure (Cluster) OpenMP]
- no silver bullet, i.e., each parallelization scheme has its problems

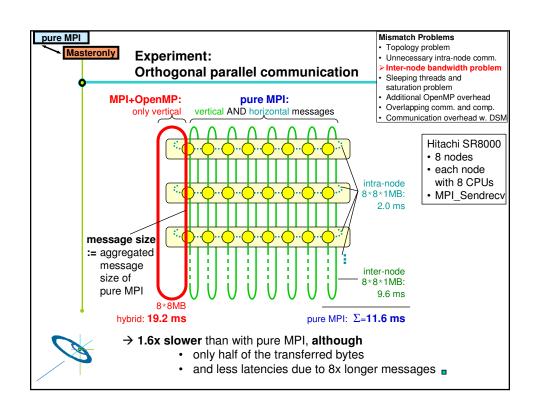


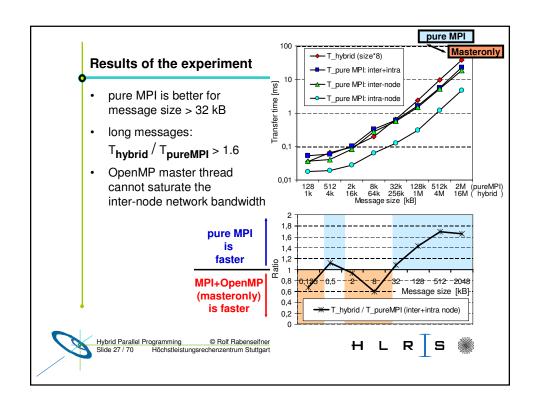


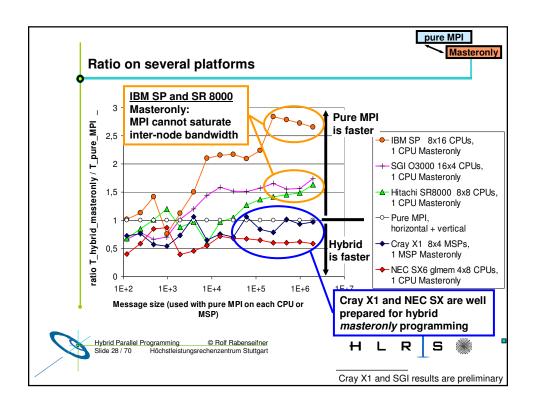












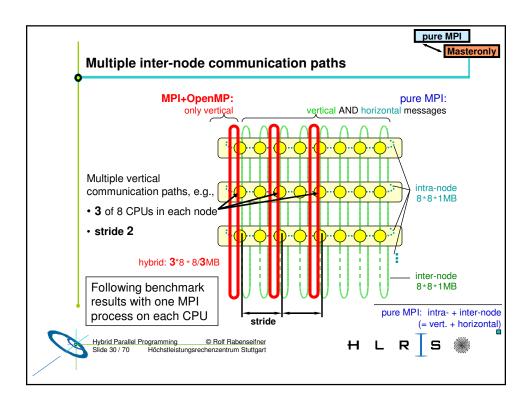


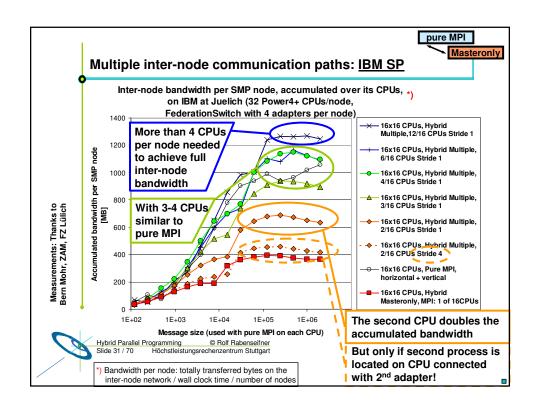
pure MPI

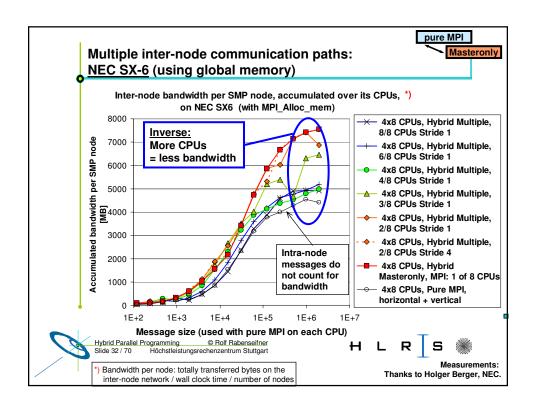
- - is one CPU able to saturate the inter-node network?
- Software:
 - internal MPI buffering may cause additional memory traffic → memory bandwidth may be the real restricting factor?
- → Let's look at parallel bandwidth results

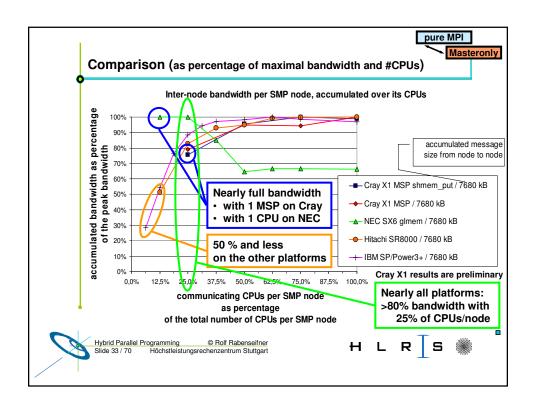


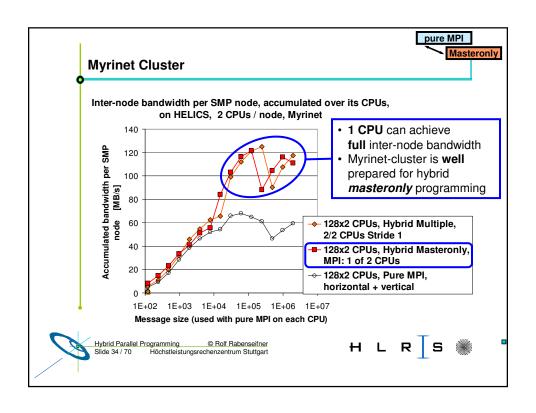












Inter-node bandwidth problem -**Summary and Work-around**

With (typically) more than 4 threads / MPI process inter-node communication network cannot be saturated

→ On constellation type systems

(more than 4 CPUs per SMP node)

- With (typically) more than 4 threads / MPI process inter-node communication network cannot be saturated
- Several multi-threaded MPI process on each SMP node
- Other problems come back:
 - · Topology problem:
 - those processes should work on neighboring domains
 - to minimize inter-node traffic
 - · Unnecessary intra-node communication between these processes
 - instead of operating on common shared memory
 - but less intra-node communication than with pure MPI



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Mismatch Problems Topology problem

Sleeping threads and saturation problem Additional OpenMP overhead Overlapping comm. and comp. Communication overhead w. DSN

· Unnecessary intra-node comm. Inter-node bandwidth problem

Mismatch Problems Topology problem Unnecessary intra-node comm.

> Inter-node bandwidth prob

Additional OpenMP overhead Overlapping comm. and comp.

Communication overhead w. DSM

Sleeping threads and saturation problem



The sleeping-threads and the saturation problem

- Masteronly:
 - all other threads are sleeping while master thread calls MPI
 - → wasting CPU time
 - →→→ wasting plenty of CPU time if master thread cannot saturate the inter-node network
- Pure MPI:
 - all threads communicate, but already 1-3 threads could saturate the network → wasting CPU time
- Overlapping communication and computation







Additional OpenMP Overhead

- Thread fork / join
- Cache flush
 - synchronization between data source thread and communicating thread implies → a cache flush
- Amdahl's law for each level of parallelism

Mismatch Problems

- Topology problem
- Unnecessary intra-node comm.
- Inter-node bandwidth problem Sleeping threads and saturation problem
- Additional OpenMP overhead
- · Overlapping comm. and comp.
- Communication overhead w. DSM





Mismatch Problems

Topology problem

Unnecessary intra-node communication

Inter-node bandwidth problem

Sleeping threads and saturation problem

Additional OpenMP overhead

- Thread fork / join

Cache flush (data source thread – communicating thread – sync. → flush)

Overlapping communication and computation [with hybrid MPI+OpenMP]

- → separation of local or halo-based code an application problem
- a programming problem → thread-ranks-based vs. OpenMP work-sharing
- a load balancing problem, if only some threads communicate / compute
- Communication overhead with DSM [with pure (Cluster) OpenMP]
- → no silver bullet, i.e., each parallelization scheme has its problems







[with pure MPI]

[with pure MPI]

[with masteronly]

[with pure MPI]

[with hybrid MPI+OpenMP]

[with hybrid MPI+OpenMP]





Overlapping Communication and Computation

MPI communication by one or a few threads while other threads are computing

- the application problem:
 - one must separate application into:
 - · code that can run before the halo data is received
 - · code that needs halo data

→ very hard to do !!!

- the thread-rank problem:
 - comm. / comp. via thread-rank
 - cannot use work-sharing directives
 - > loss of major OpenMP support
- the load balancing problem

```
if (my_thread_rank < 1) {
  MPI Send/Recv....
} else {
  my_range = (high-low-1) / (num_threads-1) + 1;
  my_low = low + (my_thread_rank+1)*my_range;
  my_high=high+ (my_thread_rank+1+1)*my_range;
  my_high = max(high, my_high)
  for (i=my_low; i<my_high; i++) {
 }
```



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Overlapping Communication and Computation

MPI communication by one or a few threads while other threads are computing

Subteams

Important proposal for OpenMP 3.x or OpenMP 4.x

Barbara Chapman et al.: Toward Enhancing OpenMP's Work-Sharing Directives. In proceedings, W.E. Nagel et al. (Eds.): Euro-Par 2006, LNCS 4128, pp. 645-654, 2006.

```
#pragma omp parallel
#pragma omp single onthreads(0)
   MPI_Send/Recv....
#pragma omp for onthreads( 1 : omp_get_numthreads()-1 )
  for (.....)
  { /* work without halo information */
  } /* barrier at the end is only inside of the subteam ^*/
#pragma omp barrier
#pragma omp for
  for (.....)
  { /* work based on halo information */
  }
} /*end omp parallel */
```

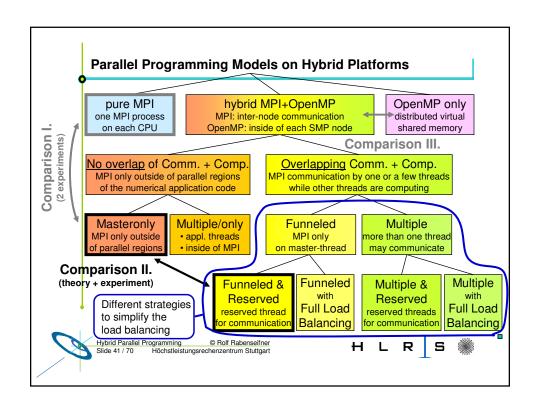


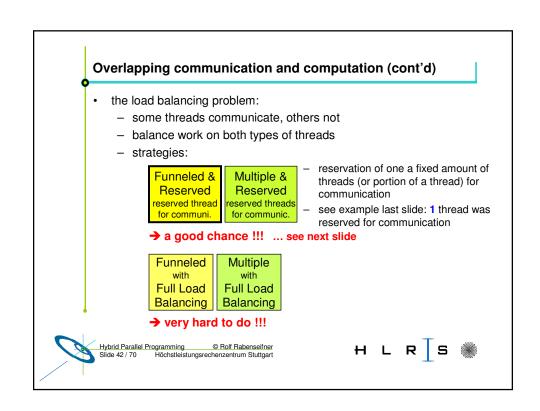
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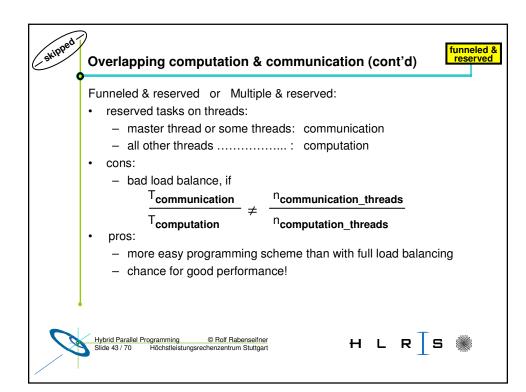
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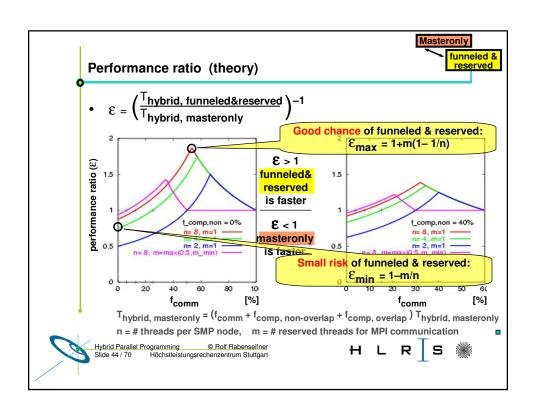


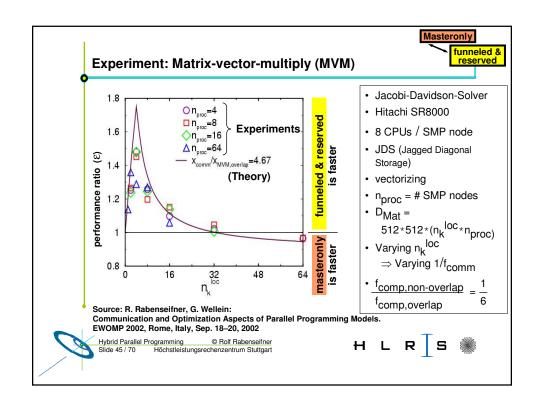


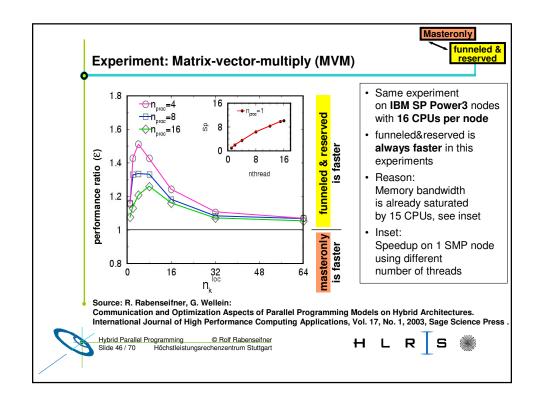


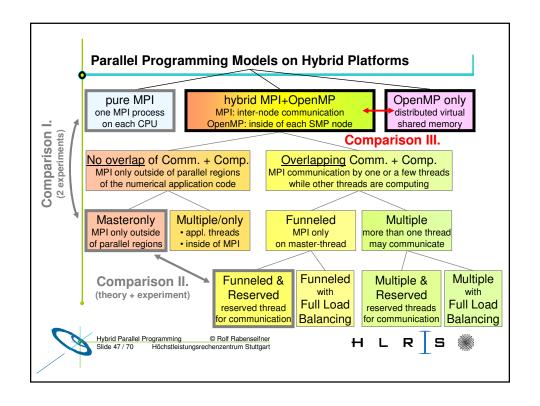


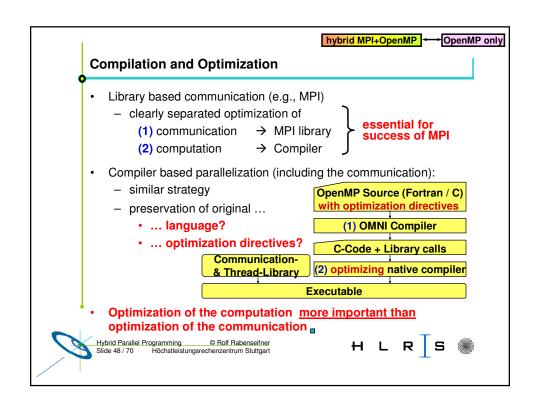












OpenMP only

OpenMP/DSM

- Distributed shared memory (DSM) //
- Distributed virtual shared memory (DVSM) //
- Shared virtual memory (SVM)
- Principles
 - emulates a shared memory
 - on distributed memory hardware
- Implementations
 - e.g., Intel® Cluster OpenMP



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Intel® Compilers with Cluster OpenMP

Goals

- To run OpenMP parallel applications on clusters
- Ease of OpenMP parallelization on cheap clusters
- Instead of
 - expensive MPI parallelization, or
 - expensive shared memory / ccNUMA hardware



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Intel® Compilers with Cluster OpenMP - Consistency Protocol

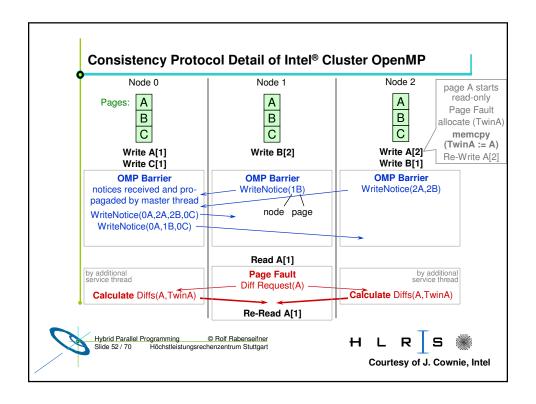
Basic idea:

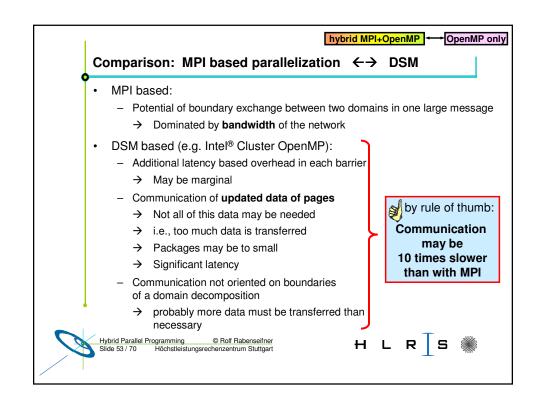
- Between OpenMP barriers, data exchange is not necessary, i.e., visibility of data modifications to other threads only after synchronization.
- When a page of sharable memory is not up-to-date, it becomes *protected*.
- Any access then faults (SIGSEGV) into Cluster OpenMP runtime library, which requests info from remote nodes and updates the page.
- Protection is removed from page.
- Instruction causing the fault is re-started, this time successfully accessing the data.

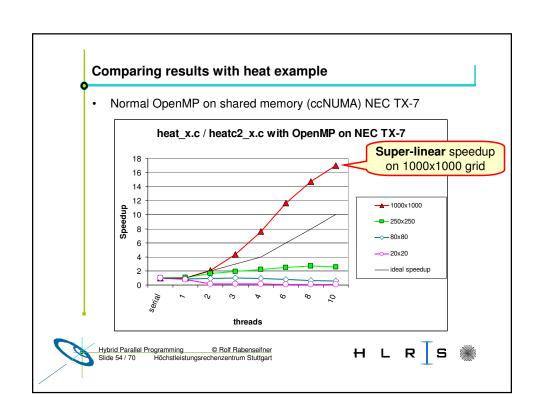


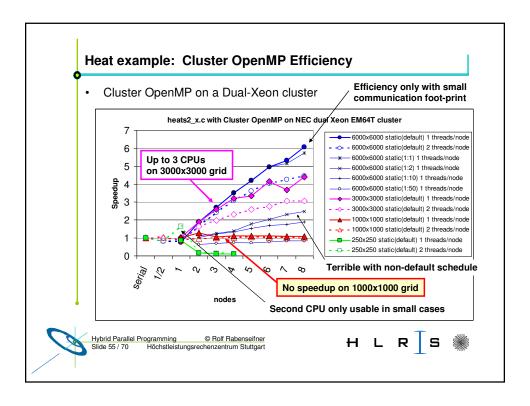


OpenMP only









Cluster OpenMP - a summary

- Intel® Cluster OpenMP can be used for programs with small communication foot-print!
- Source code modification needed: shared variables must be allocated in **sharable** memory
- · It works!
- But efficiency strongly depends on type of application!

For the appropriate application a suitable tool!





Mismatch Problems

Topology problem [with pure MPI]

Unnecessary intra-node communication [with pure MPI]

Inter-node bandwidth problem [with hybrid MPI+OpenMP]

Sleeping threads and [with masteronly] saturation problem [with pure MPI]

Additional OpenMP overhead [with hybrid MPI+OpenMP]

Thread startup / join

Cache flush (data source thread - communicating thread - sync. → flush)

Overlapping communication and computation [with hybrid MPI+OpenMP]

 an application problem → separation of local or halo-based code

– a programming problem → thread-ranks-based vs. OpenMP work-sharing

- a load balancing problem, if only some threads communicate / compute

→ no silver bullet, i.e., each parallelization scheme has its problems



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Communication overhead with DSM





[with pure (Cluster) OpenMP]





No silver bullet

- The analyzed programming models do not fit on hybrid architectures
 - whether drawbacks are minor or major
 - > depends on applications' needs
 - problems ...
 - > to utilize the CPUs the whole time
 - > to achieve the full inter-node network bandwidth
 - > to minimize inter-node messages
 - to prohibit intra-node
 - message transfer,
 - synchronization and
 - balancing (idle-time) overhead
 - > with the programming effort





Chances for optimization

- with hybrid masteronly (MPI only outside of parallel OpenMP regions), e.g.,
 - > Minimize work of MPI routines, e.g.,
 - application can copy non-contiguous data into contiguous scratch arrays (instead of using derived datatypes)
 - > MPI communication parallelized with multiple threads to saturate the inter-node network
 - by internal parallel regions inside of the MPI library
 - by the user application
 - > Use only hardware that can saturate inter-node network with 1 thread
 - > Optimal throughput:
 - reuse of idling CPUs by other applications
- On constellations:
 - > Hybrid Masteronly with several MPI multi-threaded processes on each SMP node



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Summary of mismatch problems

Performance and Programming Problems with	Pure MPI	Master- only 1 process per node	Master- only several processes per node	Over- lapping 1 process per node	Over- lapping several processes per node	Pure OpenMP: e.g., Intel Cluster OpenMP
Application topology problem (neighbor domains inside of SMP node)	4		4		4	4
Additional MPI communication inside of SMP nodes	4		4		4	
Do we achieve full inter-node bandwidth on constellations?		444		4		444
Sleeping CPUs while MPI communication	(4)	44	4			4
Additional OpenMP overhead		4	4	4	4	
Separation of (a) halo data and (b) inner data based calculations				44	44	
OpenMP work sharing only partially usable				44	44	
Load balancing problem due to hybrid programming model				4	4	

Outline

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- · Programming models on clusters of SMP nodes
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- · Thread-safety quality of MPI libraries
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MPI rules with OpenMP / Automatic SMP-parallelization

Special MPI-2 Init for multi-threaded MPI processes:

- REQUIRED values (increasing order):
 - MPI_THREAD_SINGLE: Only one thread will execute
 - THREAD_MASTERONLY: (virtual value, not part of the standard)
- MPI processes may be multi-threaded, but only master thread will make MPI-calls AND only while other threads are sleeping
- MPI_THREAD_FUNNELED: Only master thread will make MPI-calls
 MPI_THREAD_SERIALIZED: Multiple threads may make MPI-calls,
- but only one at a time
- MPI_THREAD_MULTIPLE: Multiple threads may call MPI, with no restrictions
- returned provided may be less than REQUIRED by the application





Calling MPI inside of OMP MASTER

- Inside of a parallel region, with "OMP MASTER"
- Requires MPI THREAD FUNNELED, i.e., only master thread will make MPI-calls
- Caution: There isn't any synchronization with "OMP MASTER"! Therefore, "OMP BARRIER" normally necessary to guarantee, that data or buffer space from/for other threads is available before/after the MPI call!

```
!$OMP BARRIER
!$OMP MASTER
      call MPI_Xxx(...)
!$OMP END MASTER
!$OMP BARRIER
```

#pragma omp barrier #pragma omp master MPI_Xxx(...);

#pragma omp barrier

- But this implies that all other threads are sleeping!
- The additional barrier implies also the necessary cache flush!



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... the barrier is necessary - example with MPI Recv

```
!$OMP PARALLEL
!$OMP DO
     do i=1,1000
       a(i) = buf(i)
     end do
!SOMP END DO NOWAIT
!$OMP BARRIER
!$OMP MASTER
     call MPI RECV(buf,...)
!$OMP END MASTER
!$OMP BARRIER
!$OMP DO
     do i=1,1000
       c(i) = buf(i)
     end do
!$OMP END DO NOWAIT
!$OMP END PARALLEL
```

```
#pragma omp parallel
#pragma omp for nowait
    for (i=0; i<1000; i++)
        a[i] = buf[i];
#pragma omp barrier
#pragma omp master
        MPI Recv(buf,...);
#pragma omp barrier
#pragma omp for nowait
    for (i=0; i<1000; i++)
        c[i] = buf[i];
/* omp end parallel */
```







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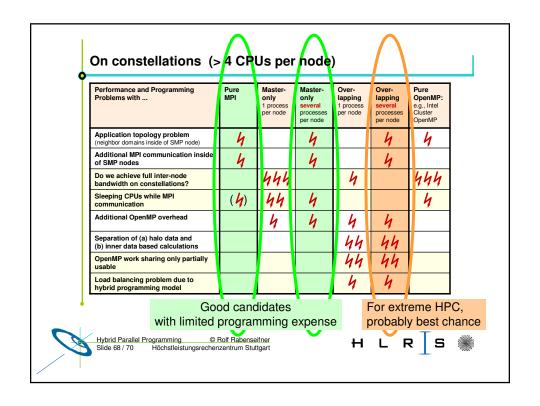
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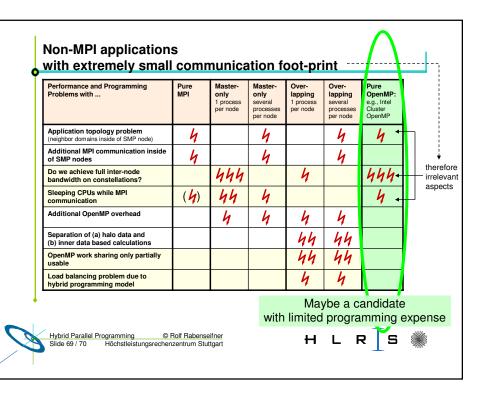
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 - Matthias Müller, HLRS
 - my colleges at HLRS

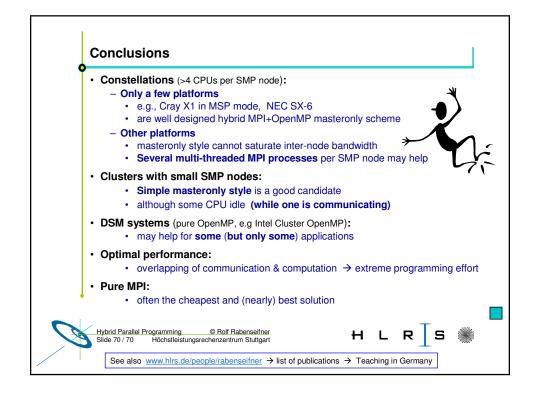




Performance and Programming Problems with		Pure MPI	Master- only 1 process per node	S	Master- only several processes per node	Over- lapping 1 process per node	Over- lapping several processes per node	Pure OpenMP: e.g., Intel Cluster OpenMP
Application topology problem (neighbor domains inside of SMP node)	П	4		١	4		4	4
Additional MPI communication insider		4			4		4	
Do we achieve full inter-node bandwidth on constellations?		,	bhh	Ī	ĺ	*	,	444
Sleeping CPUs while MPI communication		(4)	(1/4)	Ī	4			4
Additional OpenMP overhead			4	Ī	4	4	4	
Separation of (a) halo data and (b) inner data based calculations	Ī			Ĭ		44	44	
OpenMP work sharing only partially usable	١					44	44	
Load balancing problem due to hybrid programming model						4	4	
with limit			ındidate rammin			nse		







Appendix

- Abstract
- Intel® Compilers with Cluster OpenMP Consistency Protocol – Examples
- Author
- References (with direct relation to the content of this tutorial)
- · Further references



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Abstract

Abstract. Most HPC systems are clusters of shared memory nodes. Such systems can be PC clusters with dual or quad boards, but also "constellation" type systems with large SMP nodes. Parallel programming must combine the distributed memory parallelization on the node interconnect with the shared memory parallelization inside of each node.

This lecture analyzes the strength and weakness of several parallel programming models on clusters of SMP nodes. Various hybrid MPI+OpenMP programming models are compared with pure MPI. Benchmark results of several platforms are presented. A hybrid-masteronly programming model can be used more efficiently on some vector-type systems, but also on clusters of dual-CPUs. On other systems, one CPU is not able to saturate the inter-node network and the commonly used masteronly programming model suffers from insufficient inter-node bandwidth. The thread-safety quality of MPI libraries is also discussed.

Another option is the use of distributed virtual shared-memory technologies which enable the utilization of "near-standard" OpenMP on distributed memory architectures. The performance issues of this approach and its impact on applications are discussed. This lecture analyzes strategies to overcome typical drawbacks of easily usable programming schemes on clusters of SMP nodes.





Intel® Compilers with Cluster OpenMP – Real consistency protocol is more complicated

- · Diffs are done only when requested
- Several diffs are locally stored and transferred later if a thread first reads a page after several barriers.
- Each write is internally handled as a read followed by a write.
- If too many diffs are stored, a node can force a "reposession" operation, i.e., the page is marked as invalid and fully re-send if needed.
- Another key point:
 - After a page has been made read/write in a process, no more protocol traffic is generated by the process for that page until after the next synchronization (and similarly if only reads are done once the page is present for read).
 - This is key because it's how the large cost of the protocol is averaged over many accesses.
 - I.e., protocol overhead only "once" per barrier
- · Examples in the Appendix



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Courtesy of J. Cownie, Intel

Intel® Compilers with Cluster OpenMP – Consistency Protocol – Examples

Notation

• ..=A[i] Start/End Start/end a read on element i on page A

• A[i]=.. Start/End Start/end a write on element i on page A,

trap to library

Twin(A) Create a twin copy of page A

WriteNotice(A) Send write notice for page A to other processors

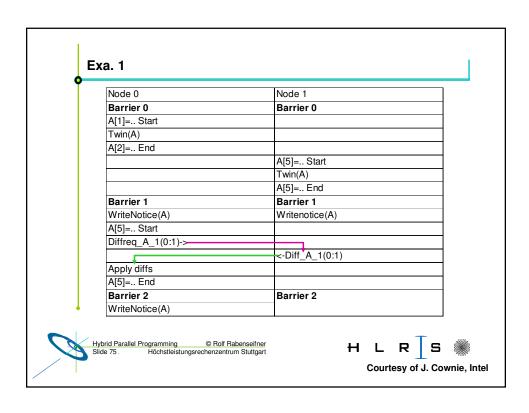
DiffReq_A_n(s:f) Request diffs for page A from node n between s and f

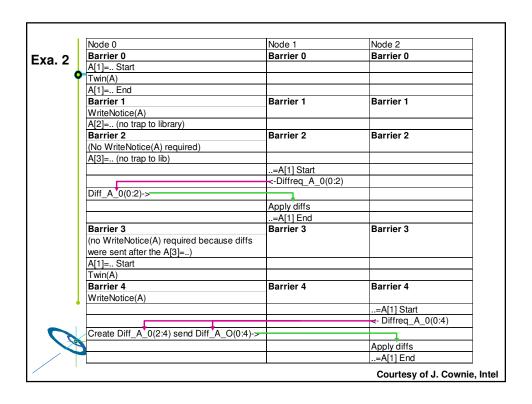
• Diff_A_n(s:f) Generate a diff for page A in writer n between s and

where s and f are barrier times. This also frees the twin for page A.

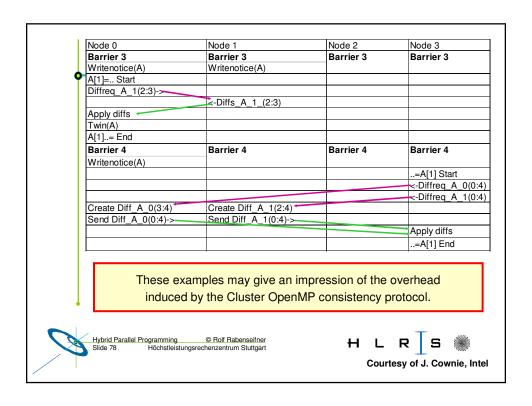








Node 0	Node 1	Node 2	Node 3
Barrier 0	Barrier 0	Barrier 0	Barrier (
A[1]= Start	A[5]= Start		
Twin(A)	Twin(A)		
A[1]= End	A[5]= End		
Barrier 1	Barrier 1	Barrier 1	Barrier 1
WriteNotice(A)	WriteNotice(A)		
A[2]= Start	A[1]= Start		
Diffreq_A_1(0:1)->	<-Diffreq_A_0(0:1)		
Diff_A_0(0:1)->	<-Diff_A_1_(0:1)		
Apply diff	Apply diff		
Twin(A)	Twin(A)		
A[2]= End	A[1]= End		
Barrier 2	Barrier 2	Barrier 2	Barrier 2
WriteNotice(A)	WriteNotice(A)		
A[3]= Start	A[6]= Start		
Diffreq_A_1(1:2)->	<-Diffreq_A_A(1:2)		
Diffs_A_0(1:2)	<-Diffs_A_1(1:2)		
Apply diffs	Apply diffs		
Twin(A)	Twin(A)		
A[3]= End	A[6]= End		
		=A[1] Start	
		<-Diffreq_A_1(0:2)	
Create Diff A 0(1:2)	Create Diff A 1(1:2)		
Send Diff_A_0(0:2)->	Send Diff_A_1(0:2)->-		
		Apply all diffs	
		=A[1] End	



Rolf Rabenseifner



Dr. Rolf Rabenseifner studied mathematics and physics at the University of Stuttgart. Since 1984, he has worked at the High-Performance Computing-Center Stuttgart (HLRS). He led the projects DFN-RPC, a remote procedure call tool, and MPI-GLUE, the first metacomputing MPI combining different vendor's MPIs without loosing the full MPI interface. In his dissertation, he developed a controlled logical clock as global time for trace-based profiling of parallel and distributed applications. Since 1996, he has been a member of the MPI-2 Forum. From January to April 1999, he was an invited researcher at the Center for High-Performance Computing at Dresden University of Technology.

Currently, he is head of Parallel Computing - Training and Application Services at HLRS. He is involved in MPI profiling and benchmarking, e.g., in the HPC Challenge Benchmark Suite. In recent projects, he studied parallel I/O, parallel programming models for clusters of SMP nodes, and optimization of MPI collective routines. In workshops and summer schools, he teaches parallel programming models in many universities and labs in Germany.





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