Parallel Programming Models on Hybrid Systems

MPI + OpenMP and other models on clusters of SMP nodes

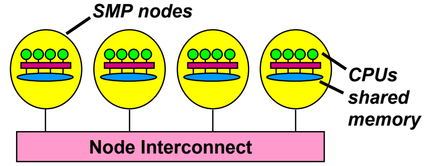
Rolf Rabenseifner
rabenseifner@hlrs.de

University of Stuttgart
High-Performance Computing-Center Stuttgart (HLRS)
www.hlrs.de

Outline

Motivation

- HPC systems
  - often clusters of SMP nodes
  - i.e., hybrid architectures



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

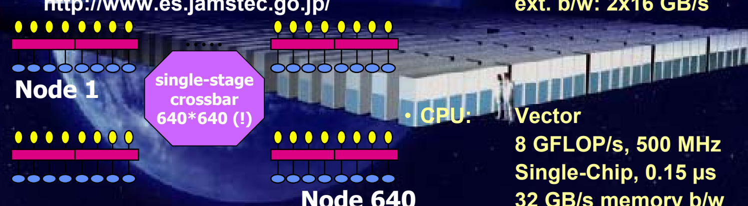
} **optimal usage of the hardware**

- Appropriate parallel programming models / Pros & Cons

Earth Simulator Project ESRDC / GS 40 (NEC)

- Virtual Earth - simulating
  - Climate change (global warming)
  - El Niño, hurricanes, droughts
  - Air pollution (acid rain, ozone hole)
  - Diastrophism (earthquake, volcanism)
- Installation: 2002
  http://www.es.jamstec.go.jp/

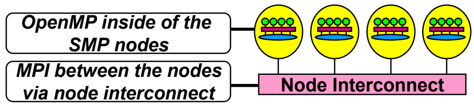
- System: 640 nodes, 40 TFLOP/s
  10 TB memory
  optical 640x640 crossbar
  50m x 20m without peripherals
- Node: 8 CPUs, 64 GFLOP/s
  16 GB, SMP
  ext. b/w: 2x16 GB/s



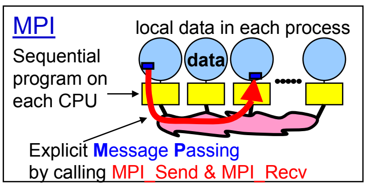
- CPU: Vector
  8 GFLOP/s, 500 MHz
  Single-Chip, 0.15 µs
  32 GB/s memory b/w

Major Programming models on hybrid systems

- Pure MPI (one MPI process on each CPU)
- Hybrid MPI+OpenMP
  - shared memory OpenMP
  - distributed memory MPI

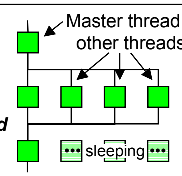


- Other: Virtual shared memory systems, HPF, …
- Often **hybrid programming (MPI+OpenMP)** slower than **pure MPI**
  - why?



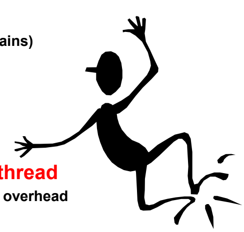
OpenMP (shared data)

some_serial_code
#pragma omp parallel for
for (j=…;…; j++)
block_to_be_parallelized
again_some_serial_code



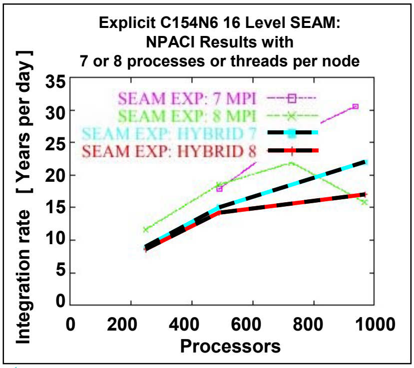
But results may surprise!

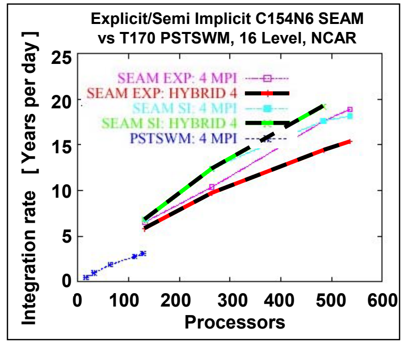
- Example code - HYDRA
- Domain-decomposed hydrodynamics
  - (almost) independent mesh domains with ghost cells on boundaries
  - ghost cells communicate boundary information ~40-50 times per cycle
- Parallelism model: single level
  - MPI divides domains among compute nodes
  - OpenMP further subdivides domains among processors
  - domain size set for cache efficiency
    - **minimizes memory usage, maximizes efficiency**
    - **scales to very large problem sizes (>10^7 zones, >10^3 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**



Example from SC 2001

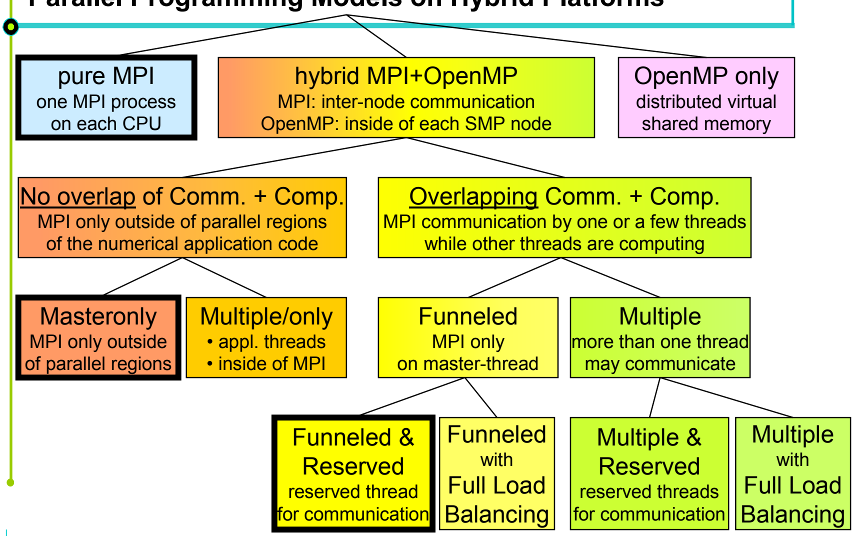
- Pure MPI versus
  Hybrid MPI+OpenMP (Masteronly)
- What's better?
  → it depends on?





Figures: Richard D. Loft, Stephen J. Thomas, John M. Dennis:
Terascale Spectral Element Dynamical Core for Atmospheric General Circulation Models.
Proceedings of SC2001, Denver, USA, Nov. 2001.
http://www.sc2001.org/papers/pap.pap189.pdf
Fig. 9 and 10.

Parallel Programming Models on Hybrid Platforms



MPI rules with OpenMP / Automatic SMP-parallelization (2)

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

```
int MPI_Init_thread(int * argc, char *((*argv)[ ]), int required, int* provided)
MPI_INIT_THREAD(REQUIRED, PROVIDED, IERROR )
```

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

… the barrier is necessary – example with MPI_Recv

```
!$OMP PARALLEL
!$OMP DO
        do i=1,1000
           a(i) = buf(i)
        end do
!$OMP END DO NOWAIT
!$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 parallel
{
#pragma 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 for
nowait   for (i=0; i<1000;
i++)       c[i] = buf[i];

}
#pragma end parallel
```


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

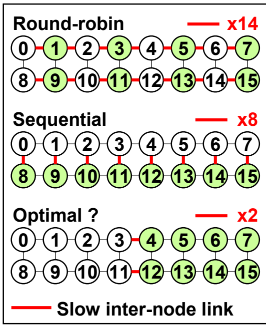
→ **no silver bullet**
  - **each parallelization scheme has its problems**

The Topology Problem with Pure MPI

- ➢ **Topology problem**
- Unnecessary intra-node comm.
- Inter-node bandwidth problem
- Sleeping threads and saturation problem
- Additional OpenMP overhead
- Overlapping comm. and comp.

pure MPI
one MPI process on each CPU

Exa.: 2 SMP nodes, 8 CPUs/node



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

Problems
- To fit application topology on hardware topology

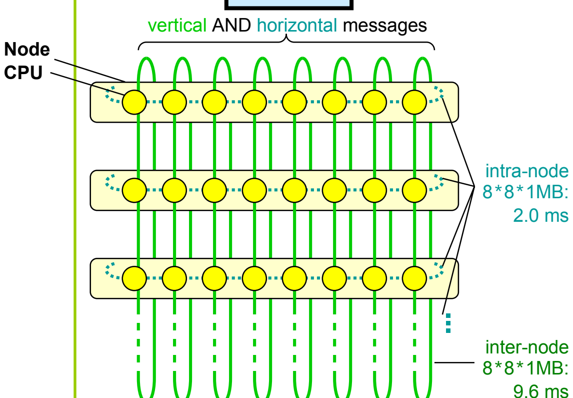
Solutions for Cartesian grids:
- E.g. choosing ranks in MPI_COMM_WORLD ???
  - **round robin (rank 0 on node 0, rank 1 on node 1, ...)**
  - **Sequential (ranks 0-7 on 1st node, ranks 8-15 on 2nd …)**

… in general
- load balancing in two steps:
  - **all cells among the SMP nodes (e.g. with ParMetis)**
  - **inside of each node: distributing the cells among the CPUs**
- or … → **using hybrid programming models**

Unnecessary intra-node communication

- Topology problem
- ➢ **Unnecessary intra-node comm.**
- Inter-node bandwidth problem
- Sleeping threads and saturation problem
- Additional OpenMP overhead
- Overlapping comm. and comp.

pure MPI



pure MPI: Σ=**11.6 ms**

Alternative:
- Hybrid MPI+OpenMP
- No intra-node messages
- Longer inter-node messages
- **Really faster ???????**
  (… wait 2 slides)

Timing:
Hitachi SR8000, MPI_Sendrecv
8 nodes, each node with 8 CPUs

Programming Models on Hybrid Platforms: Hybrid Masteronly

Masteronly
MPI only outside of parallel regions

```
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
```

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

Problems
- MPI-lib must support MPI_THREAD_FUNNELED

Disadvantages
- do we get full inter-node bandwidth? **… next slide**
- all other threads are sleeping while master thread communicates

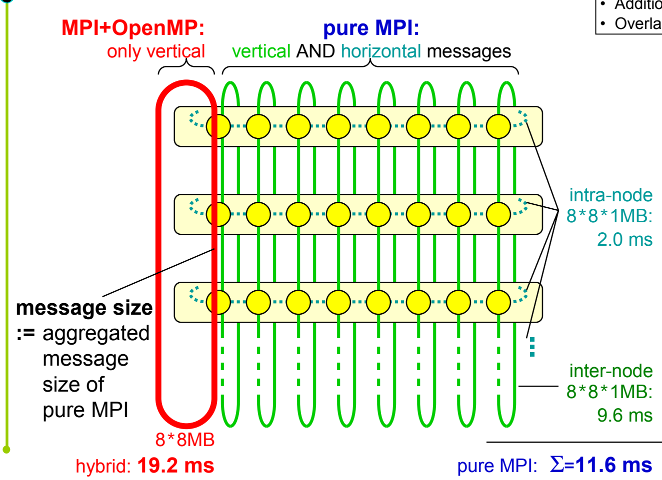
→Reason for implementing overlapping of communication & computation

pure MPI
Masteronly

Experiment: Orthogonal parallel communication

- Topology problem
- Unnecessary intra-node comm.
- ➢ **Inter-node bandwidth problem**
- Sleeping threads and saturation problem
- Additional OpenMP overhead
- Overlapping comm. and comp.

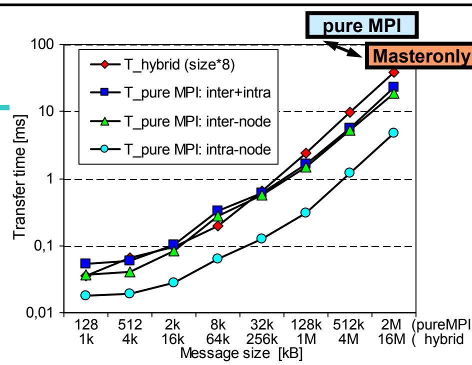
Hitachi SR8000
- 8 nodes
- each node with 8 CPUs
- MPI_Sendrecv

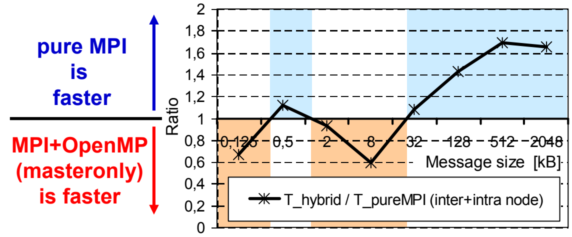


→ **1.6x slower** than with pure MPI, **although**
- only half of the transferred bytes
- and less latencies due to 8x longer messages

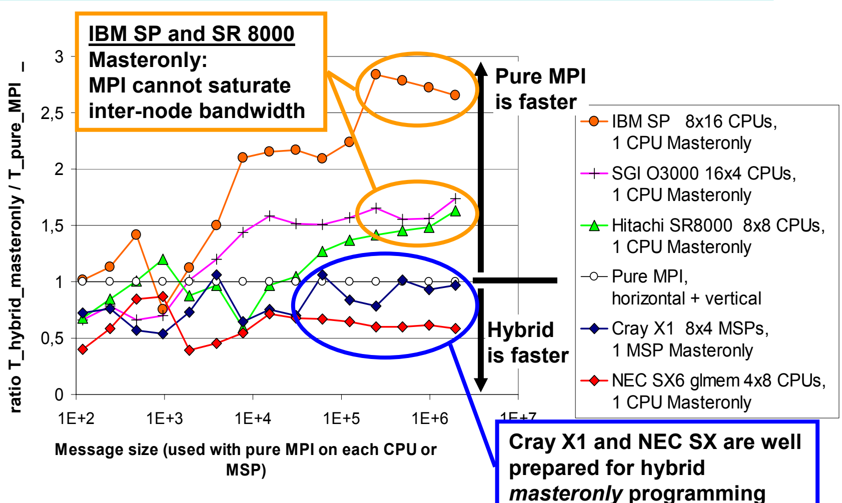
Results of the experiment

- pure MPI is better for message size > 32 kB
- long messages: $T_{\mathbf{hybrid}} / T_{\mathbf{pureMPI}} > 1.6$
- OpenMP master thread cannot saturate the inter-node network bandwidth





Ratio on several platforms



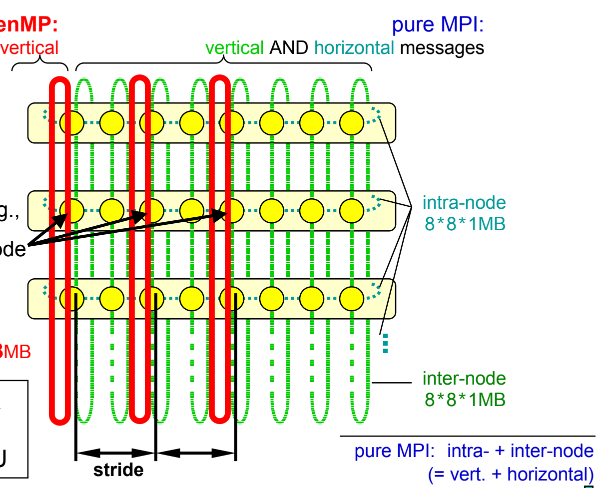
Cray X1 and SGI results are preliminary

Possible Reasons

- Hardware:
  – 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**

Multiple inter-node communication paths



Multiple vertical communication paths, e.g.,

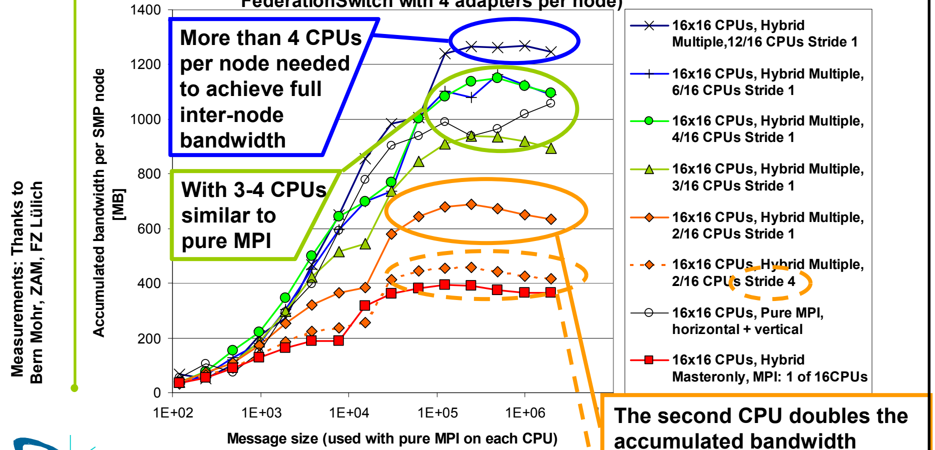
- **3** of 8 CPUs in each node
- **stride 2**

hybrid: **3***8 * 8/**3**MB

Following benchmark results with one MPI process on each CPU

Multiple inter-node communication paths: IBM SP

Inter-node bandwidth per SMP node, accumulated over its CPUs, *)
on IBM at Juelich (32 Power4+ CPUs/node,
FederationSwitch with 4 adapters per node)



The second CPU doubles the accumulated bandwidth

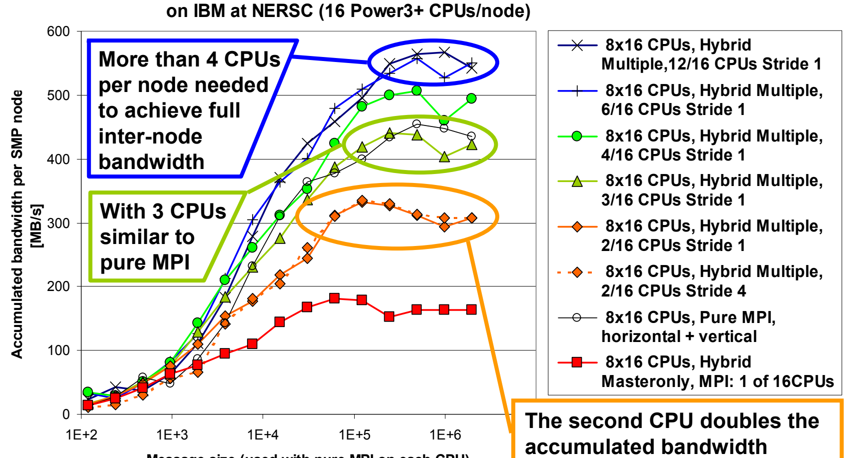
But only if second process is located on CPU connected with 2nd adapter!

*) Bandwidth per node: totally transferred bytes on the inter-node network / wall clock time / number of nodes

skipped

Multiple inter-node communication paths: IBM SP

Inter-node bandwidth per SMP node, accumulated over its CPUs, *)
on IBM at NERSC (16 Power3+ CPUs/node)



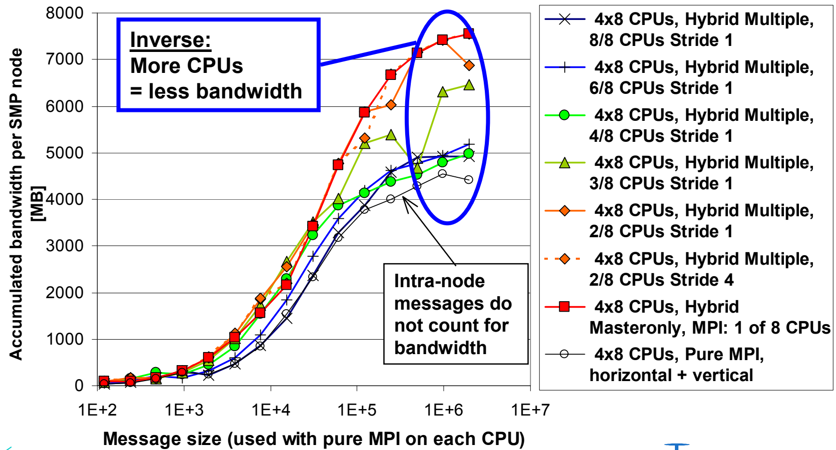
The second CPU doubles the accumulated bandwidth

*) Bandwidth per node: totally transferred bytes on the inter-node network / wall clock time / number of nodes

Measurements: Thanks to Gerhard Wellein, RRZE, and Horst Simon, NERSC.

Multiple inter-node communication paths: NEC SX-6 (using global memory)

Inter-node bandwidth per SMP node, accumulated over its CPUs, *)
on NEC SX6 (with MPI_Alloc_mem)



H L R | S

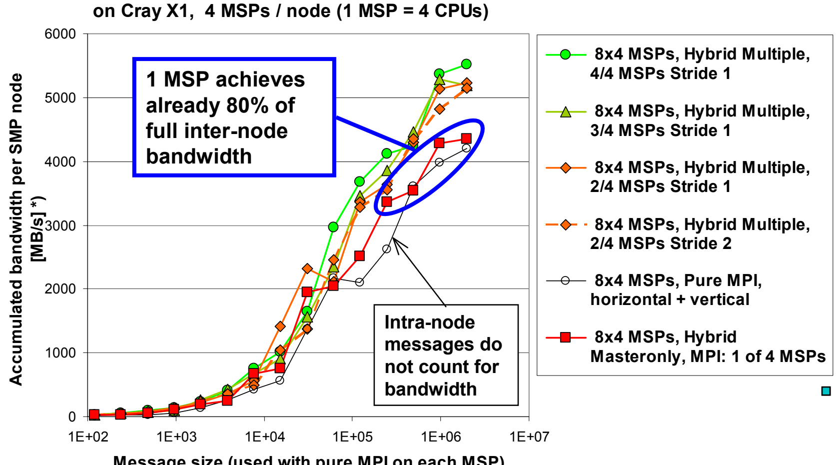
*) Bandwidth per node: totally transferred bytes on the inter-node network / wall clock time / number of nodes

Measurements:
Thanks to Holger Berger, NEC.

skipped

Multiple inter-node communication paths: Cray X1, used with 4 MSPs/node (preliminary results)

Inter-node bandwidth per SMP node, accumulated over its CPUs, *)
on Cray X1, 4 MSPs / node (1 MSP = 4 CPUs)



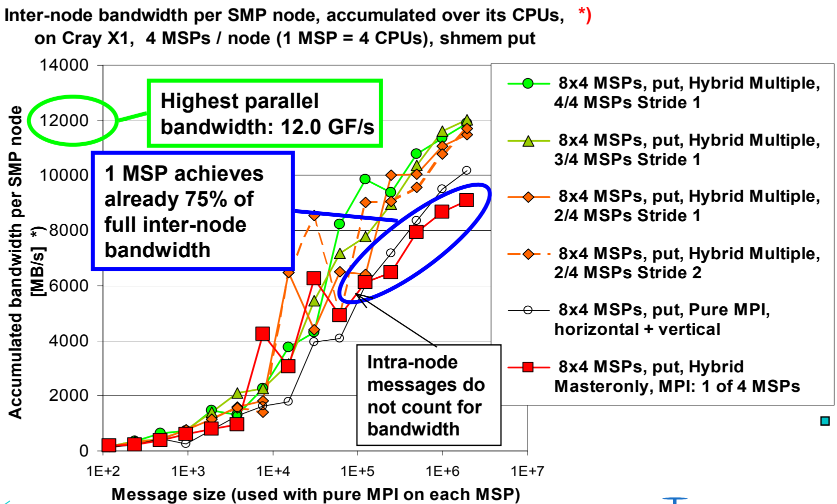
H L R | S

*) Bandwidth per node: totally transferred bytes on the inter-node network / wall clock time / number of nodes

Measurements:
Thanks to Monika Wierse and Wilfried Oed, CRAY.

skipped

Multiple inter-node communication paths: Cray X1, used with 4 MSPs/node, shmem put (instead MPI)

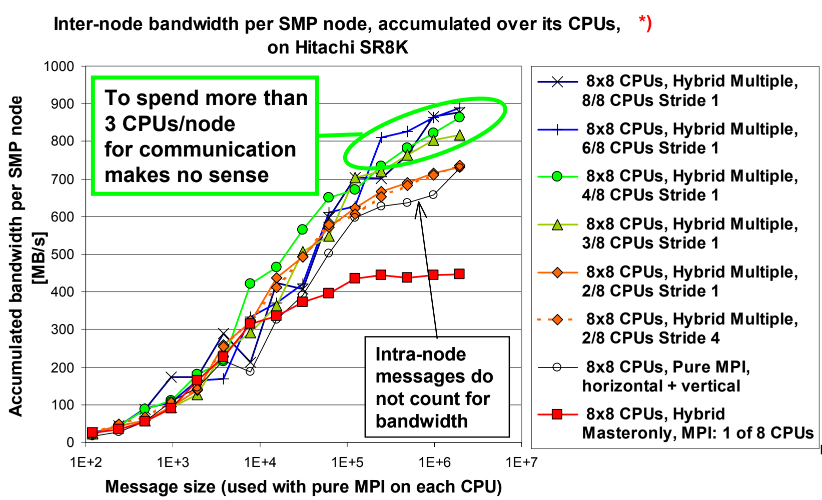


*) Bandwidth per node: totally transferred bytes on the inter-node network / wall clock time / number of nodes

Measurements:
Thanks to Monika Wierse and Wilfried Oed, CRAY.

skipped

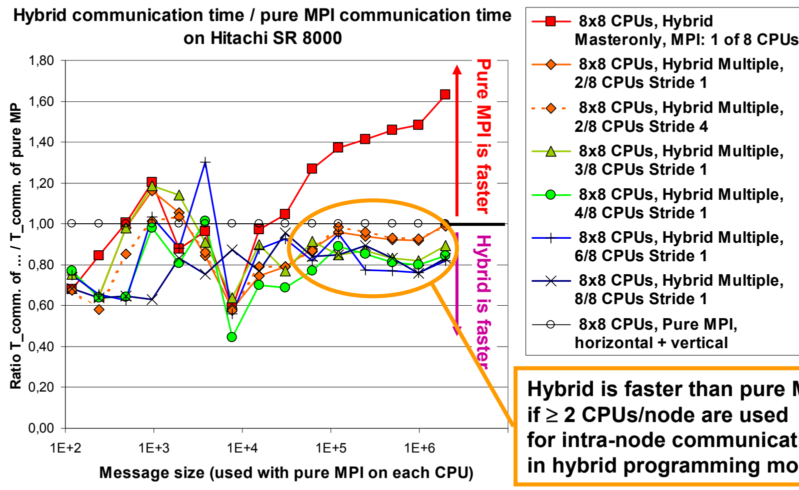
Multiple inter-node communication paths: Hitachi SR8000



*) Bandwidth per node: totally transferred bytes on the inter-node network / wall clock time / number of nodes

skipped

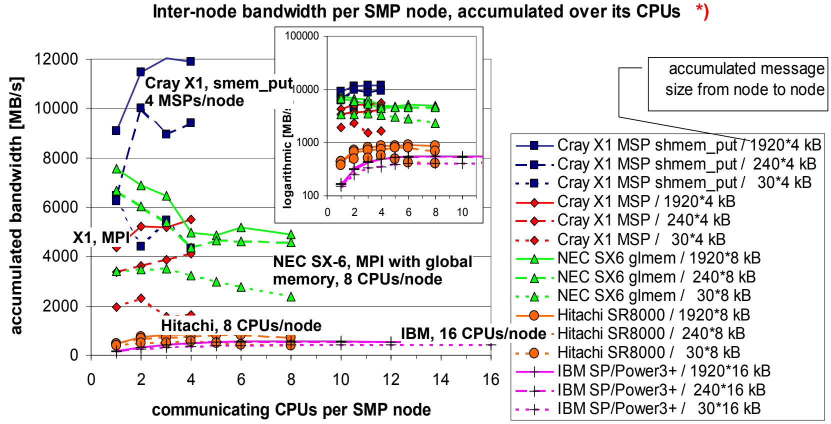
Multiple inter-node communication paths: Hitachi SR 8000



Hybrid is faster than pure MPI if ≥ 2 CPUs/node are used for intra-node communication in hybrid programming model

Comparison

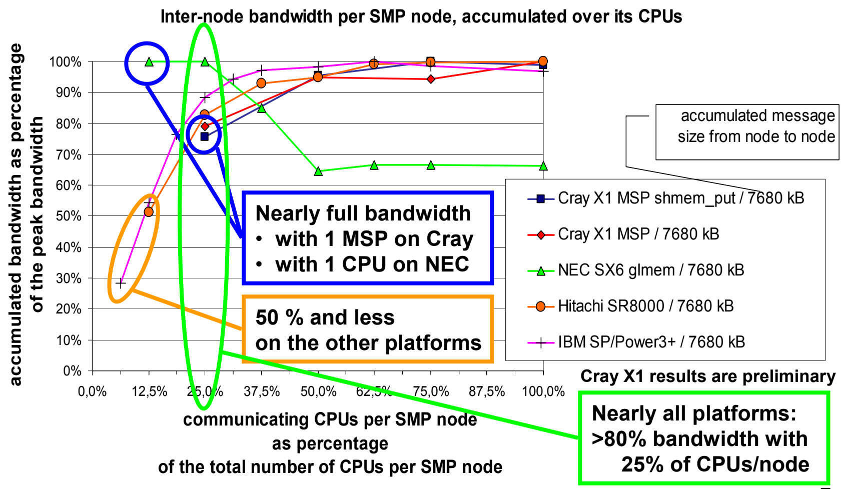
Inter-node bandwidth per SMP node, accumulated over its CPUs *)



Cray X1 results are preliminary

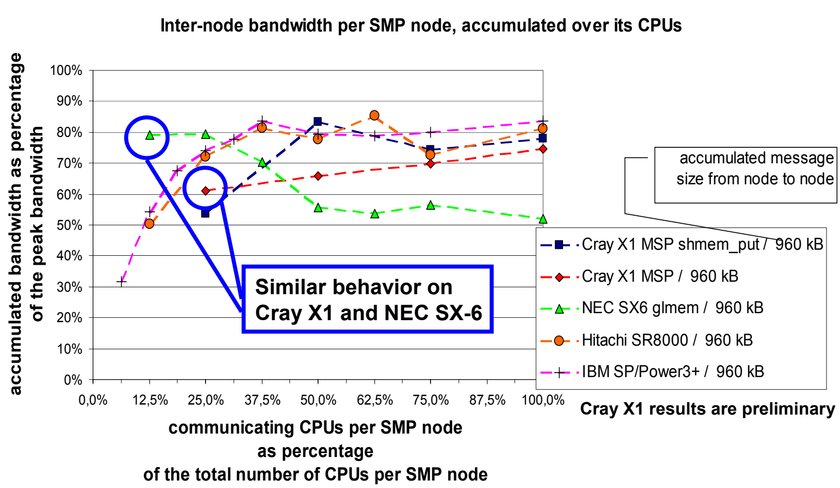
*) Bandwidth per node: totally transferred bytes on the inter-node network / wall clock time / number of nodes

Comparison (as percentage of maximal bandwidth and #CPUs)



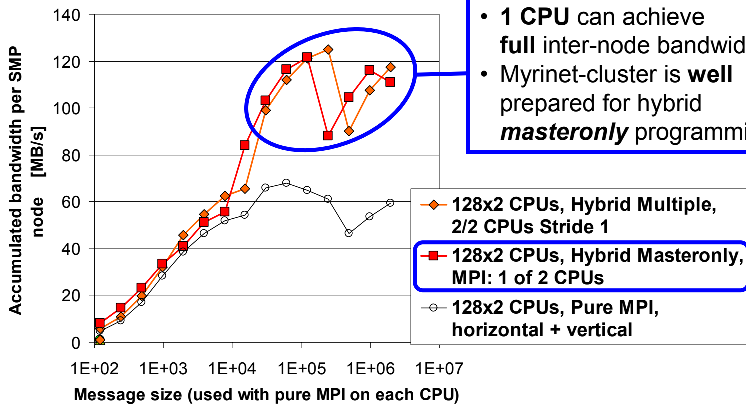
skipped

Comparison (only 960 kB aggregated message size)



Myrinet Cluster

Inter-node bandwidth per SMP node, accumulated over its CPUs, on HELICS, 2 CPUs / node, Myrinet

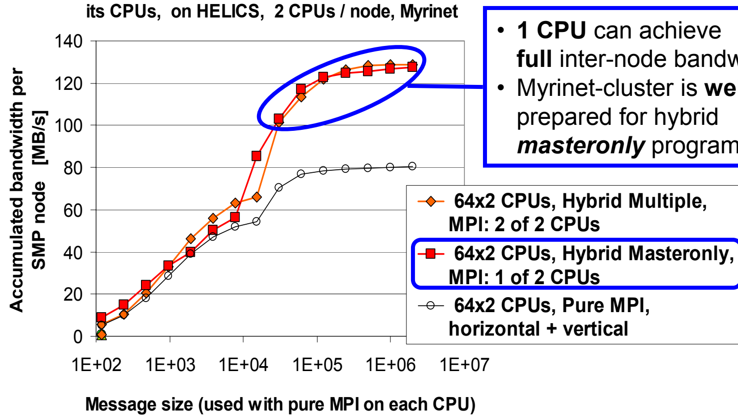


- **1 CPU** can achieve **full** inter-node bandwidth
- Myrinet-cluster is **well** prepared for hybrid ***masteronly*** programming

skipped

Myrinet Cluster (only 64 nodes)

Inter-node bandwidth per SMP node, accumulated over its CPUs, on HELICS, 2 CPUs / node, Myrinet



- **1 CPU** can achieve **full** inter-node bandwidth
- Myrinet-cluster is **well** prepared for hybrid ***masteronly*** programming

skipped

Hybrid Programming on Cray X1: MSP based usage

- pure MPI or hybrid masteronly MPI+OpenMP
  → same communication time
- 1 MSP already achieves 80% of maximum bandwidth (**contiguous data**)
  - **Are CPU-intensive MPI routines (Reduce, strided data) efficient & multi-threaded ?**
- Hybrid programming → 4 layers of parallelism

– MPI between nodes	(e.g. domain decomposition)
– OpenMP between MSPs	(e.g. outer loops)
– Automatic parallelization	(e.g. inner loops)
– Vectorization	(e.g. most inner loops)

  → risk of Amdahl's law on each level!
- Hybrid & overlapping communication and computation
  - **horrible programming interface (but standardized)**
  - **but chance to use sleeping MSPs while master MSP communicates**

skipped

Hybrid Programming on Cray X1: SSP based

- Communication is hardware-bound to SSP
  – 1 SSP can get only 1/4 of 1 MSP's inter-node bandwidth
  – with shmem put:
    all SSPs of a node can together achieve full inter-node bandwidth
    (12.3 GB/s of 12.8 GB/s hardware specification)
- Hybrid MPI+OpenMP, masteronly style
  – optimized MPI library needed with same bandwidth as on 1 or 4 MSP
  – e.g., internally thread-parallel
- Multiple communicating user-threads are not supported
- pure MPI
  – efficient MPI implementation under development

Comparing inter-node bandwidth with CPU performance

*) Bandwidth per node: totally transferred bytes on the network / number of nodes / wall clock time

All values: aggregated over one SMP nodes. *) mess. size: 16 MB +) 2 MB	Master-only, inter-node [GB/s]	pure MPI, inter-node [GB/s]	Master-only bw / max. intra-node bw	pure MPI, intra-node [GB/s]	memory bandwidth [GB/s]	**Peak** & *Linpack* performance Gflop/s	max.inter-node bw / peak & *Linpack* perf. B/Flop	nodes*CPUs
Cray X1, shmem_put preliminary results	9.27	**12.34**	**75 %**	33.0	136	**51.2** *45.03*	**0.241** *0.274*	**8 * 4 MSPs**
Cray X1, MPI preliminary results	4.52	**5.52**	**82 %**	19.5	136	**51.2** *45.03*	**0.108** *0.123*	**8 * 4 MSPs**
NEC SX-6 global memory	**7.56**	4.98	**100 %**	78.7 93.7+)	256	**64** *61.83*	**0.118** *0.122*	**4 * 8 CPUs**
NEC SX-5Be local memory	2.27	**2.50 a)**	**91 %**	35.1	512	**64** *60.50*	**0.039** *0.041*	**2 *16 CPUs** a) only with 8
Hitachi SR8000	0.45	**0.91**	**49 %**	5.0	32 store 32 load	**8** *6.82*	**0.114** *0.133*	**8 * 8 CPUs**
IBM SP Power3+	0.16	**0.57+)**	**28 %**	2.0	16	**24** *14.27*	**0.023** *0.040*	**8 *16 CPUs**
SGI O3000, 600MHz	0.43+)	**1.74+)**	**25 %**	1.73+)		**4.8** *3.64*	**0.363** *0.478*	**16 *4 CPUs**
SUN-fire (prelimi.)	0.15	**0.85**	**18 %**	1.68				**4 *24 CPUs**
HELICS Dual-PC cluster with Myrinet	0.118 +)	**0.119 +)**	**100 %**	0.104 +)		**2.80** *1.61*	**0.043** *0.074*	**128 *2 CPUs**

The sleeping-threads and the saturation problem

- Topology problem
- Unnecessary intra-node comm.
- Inter-node bandwidth problem
- ➢ **Sleeping threads and saturation problem**
- Additional OpenMP overhead
- Overlapping comm. and comp.

- 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**

Example with Sweep3d – analyzed with Kojak

- Expert: part of Kojak project at FZ Jülich,
  - Contact: Dr. Bernd Mohr
  - www.fz-jülich.de/zam/kojak/
- Sweep3d
  - ASCI Benchmark (MPI-Version)
    http://www.llnl.gov/asci_benchmarks/asci/limited/sweep3d/asci_sweep3d.html
  - A first, **insufficient** (straight-forward) hybrid "*masteronly*" MPI+OpenMP implementation
- Demo:
  - Icon starts D:\EigeneDateien\expert_Mohr\src\presenter.py
  - **File → Open →** D:\EigeneDateien\expert_Mohr\reports**sweep3d.eap.dat**
  - **Left mouse button: open more details**
  - **Right mouse double-click: choose this event class for details in next window**

Additional OpenMP Overhead

- Topology problem
- Unnecessary intra-node comm.
- Inter-node bandwidth problem
- Sleeping threads and saturation problem
- ➢ **Additional OpenMP overhead**
- Overlapping comm. and comp.

- 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 [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 fork / 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
  - **each parallelization scheme has its problems**

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 !!!**

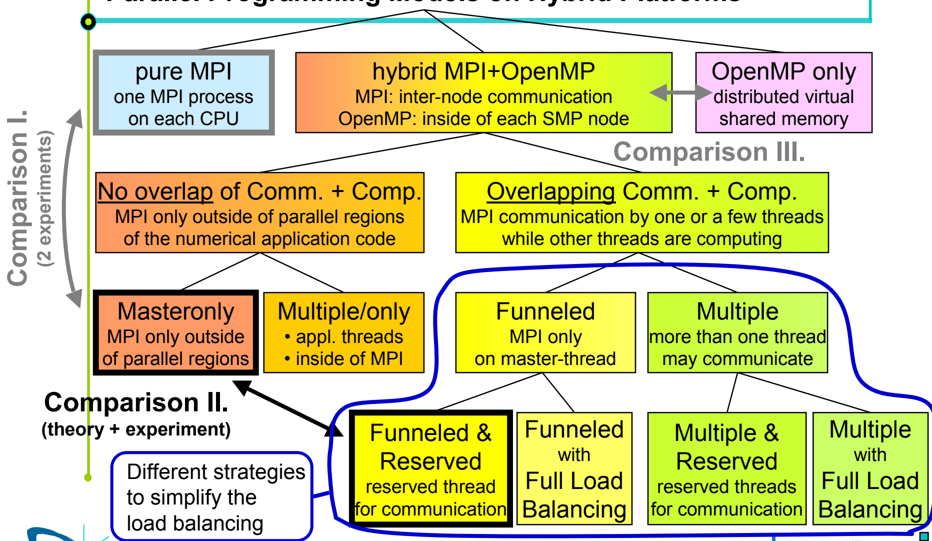
- the thread-rank problem:
  - comm. / comp. via thread-rank
  - cannot use work-sharing directives

  ➔ **loss of major OpenMP support**

```
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++) {
          ....
   }
}
```

- the load balancing problem

Parallel Programming Models on Hybrid Platforms



Overlapping communication and computation (cont'd)

- the load balancing problem:
  - some threads communicate, others not
  - balance work on both types of threads
  - strategies:

Funneled & Reserved reserved thread for communi.	Multiple & Reserved reserved threads for communic.

– reservation of one a fixed amount of threads (or portion of a thread) for communication

– see example last slide: **1** thread was reserved for communication

➔ a good chance !!! ... see next slide

Funneled with Full Load Balancing	Multiple with Full Load Balancing

➔ very hard to do !!!

funneled & reserved

Overlapping computation & communication (cont'd)

Funneled & reserved   or   Multiple & reserved:

- reserved tasks on threads:
  - master thread or some threads: communication
  - all other threads ……………... :   computation
- cons:
  - bad load balance, if

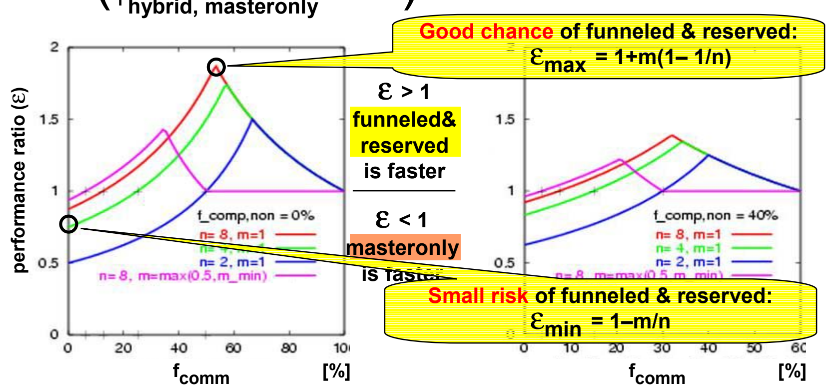
$$\frac{T_{\text{communication}}}{T_{\text{computation}}} \neq \frac{n_{\text{communication\_threads}}}{n_{\text{computation\_threads}}}$$

- pros:
  - more easy programming scheme than with full load balancing
  - chance for good performance!

Masterony ↔ funneled & reserved

Performance ratio (theory)

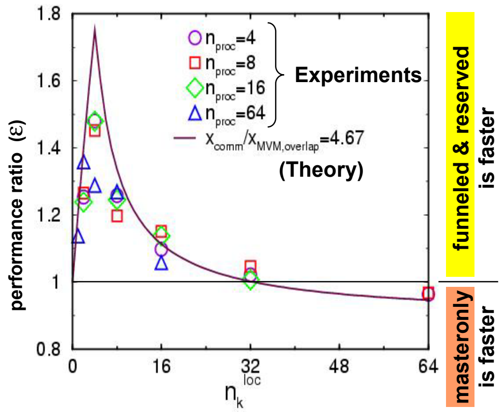
- $\varepsilon = \left(\frac{T_{\text{hybrid, funneled\&reserved}}}{T_{\text{hybrid, masteronly}}}\right)^{-1}$



$T_{\text{hybrid, masteronly}} = (f_{\text{comm}} + f_{\text{comp, non-overlap}} + f_{\text{comp, overlap}})\, T_{\text{hybrid, masteronly}}$

n = # threads per SMP node,   m = # reserved threads for MPI communication

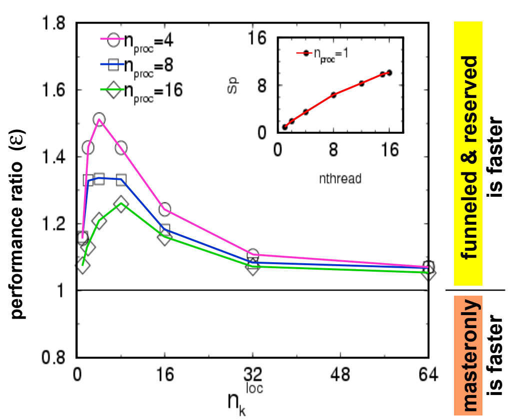
Experiment: Matrix-vector-multiply (MVM)



- Jacobi-Davidson-Solver
- Hitachi SR8000
- 8 CPUs / SMP node
- JDS (Jagged Diagonal Storage)
- vectorizing
- n_{proc} = # SMP nodes
- D_{Mat} = $512*512*(n_k^{loc}*n_{proc})$
- Varying n_k^{loc} $\Rightarrow$ Varying $1/f_{comm}$
- $\dfrac{f_{comp,non-overlap}}{f_{comp,overlap}} = \dfrac{1}{6}$

Source: R. Rabenseifner, G. Wellein:
Communication and Optimization Aspects of Parallel Programming Models.
EWOMP 2002, Rome, Italy, Sep. 18–20, 2002

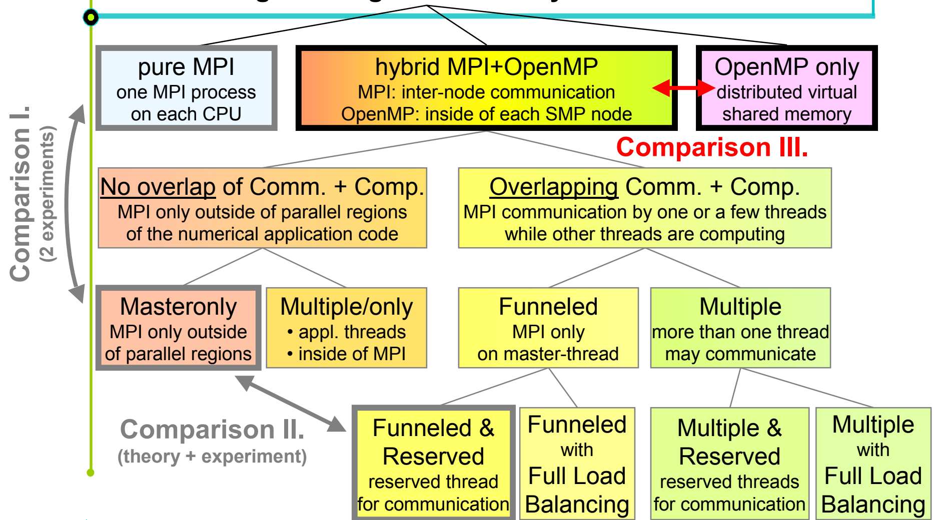
Experiment: Matrix-vector-multiply (MVM)



- Same experiment on **IBM SP Power3** nodes with **16 CPUs per node**
- funneled&reserved is **always faster** in this experiments
- Reason: Memory bandwidth is already saturated by 15 CPUs, see inset
- Inset: Speedup on 1 SMP node using different number of threads

Source: R. Rabenseifner, G. Wellein:
Communication and Optimization Aspects of Parallel Programming Models on Hybrid Architectures.
International Journal of High Performance Computing Applications, Vol. 17, No. 1, 2003, Sage Science Press .

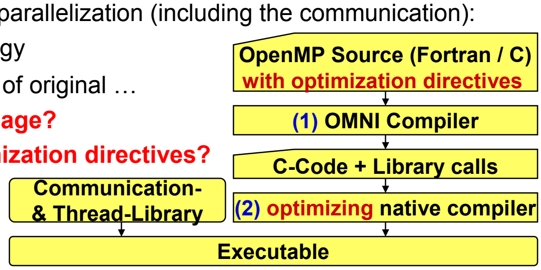
Parallel Programming Models on Hybrid Platforms



Compilation and Optimization

- Library based communication (e.g., MPI)
  - clearly separated optimization of
    - **(1)** communication → MPI library
    - **(2)** computation → Compiler

    } **essential for success of MPI**
- Compiler based parallelization (including the communication):
  - similar strategy
  - preservation of original …
    - **… language?**
    - **… optimization directives?**



- **Optimization of the computation <u>more important than</u> optimization of the communication** pure MPI ↔ 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., TreadMarks

Outline

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

skipped

Other Concepts

- Distributed memory programming (DMP) language extensions
  - Co-array Fortran
  - UPC (Unified Parallel C)

  Idea: direct access to remote data via additional [rank] index
- Multi level parallelism (MLP)
  - combining OpenMP (inside of the processes)
  - with Sys V shared memory (data access between processes)
  - only on ccNUMA

No standards!
Only on a few platforms!

skipped

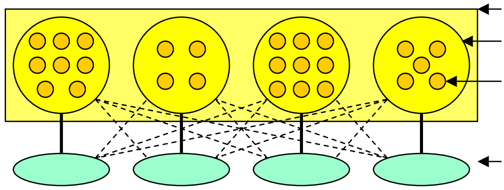
DMP Language Extensions

- Programmable access to the memory of the other processes
- Language bindings:
  - Co-array Fortran
  - UPC (Unified Parallel C)
- Special additional array index to explicitly address the process
- Examples (Co-array Fortran):

integer a[*], b[*]	! Replicate **a** and **b** on all processes
a[1] = b[6]	! **a** on process 1 := **b** on process 6
dimension (n,n) :: u[3,*]	! Allocates the n×n array **u** ! on each of the 3×* processes
p = THIS_IMAGE(u,1)	! first co-subscript of local process
q = THIS_IMAGE(u,1)	! second co-subscript of local process
u(1:n,1)[p+1,q] = u(1:n,n)[p,q]	! Copy right boundary u(**1**,) on process [**p**,] ! to right neighbor [**p+1**,] into left boundary u(**n**,)

skipped

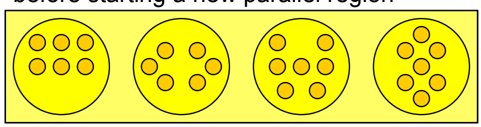
Multi Level Parallelism (MLP)



- program
- processes
- multiple threads inside of each process (**OpenMP**)
- data associated with each process
- **but shared (ccNUMA) access to other processes' data**

Cheap load balancing

- by changing the number of threads per process
- before starting a new parallel region



Acknowledgements

- I want to thank
  - Gerhard Wellein, RRZE
  - Monika Wierse, Wilfried Oed, and Tom Goozen, CRAY
  - Holger Berger, NEC
  - Reiner Vogelsang, SGI
  - Gabriele Jost, NASA
  - Dieter an Mey, RZ Aachen
  - Horst Simon, NERSC
  - Matthias Müller, HLRS
  - my colleges at HLRS

Conclusions

- **Only a few platforms**
  - e.g., Cray X1 in MSP mode, NEC SX-6, and Myrinet-cluster
  - are well designed hybrid MPI+OpenMP masteronly scheme
- **Other platforms**
  - masteronly style cannot saturate inter-node bandwidth
  - optimization chances should be used
- **Pure MPI and hybrid masteronly:**
  - idling CPUs (while one or some are communicating)
- **DSM systems** (pure OpenMP):
  - may help for some applications
- **Optimal performance:**
  - overlapping of communication & computation
    → extreme programming effort
  - optimal throughput
    → reuse of idling CPUs by other applications
    - **single threaded, vectorized, low-priority, small-medium memory needs**

See also www.hlrs.de/people/rabenseifner → list of publications