Non-Blocking Collectives for MPI

– overlap at the highest level –

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Outline

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Fundamental Assumptions (I)

We need more powerful machines!

- Solutions for real-world scientific problems need huge processing power (more than available)

Capabilities of single PEs have fundamental limits

- The scaling/frequency race is currently stagnating
- Moore's law is still valid (number of transistors/chip)
- Instruction level parallelism is limited (pipelining, VLIW, multi-scalar)

Explicit parallelism seems to be the only solution

- Single chips and transistors get cheaper
- Implicit transistor use (ILP, branch prediction) have their limits

Fundamental Assumptions (II)

Parallelism requires communication

- Local or even global data-dependencies exist
- Off-chip communication becomes necessary
- Bridges a physical distance (many PEs)

Communication latency is limited

- It's widely accepted that the speed of light limits data-transmission
- Example: minimal 0-byte latency for $1m \approx 3.3ns \approx 13$ cycles on a $4GHz$ PE

Bandwidth can hide latency only partially

- Bandwidth is limited (physical constraints)
- The problem of "scaling out" (especially iterative solvers)

Assumptions about Parallel Program Optimization

Collective Operations

- Collective Operations (COs) are an optimization tool
- CO performance influences application performance
- optimized implementation and analysis of CO is non-trivial

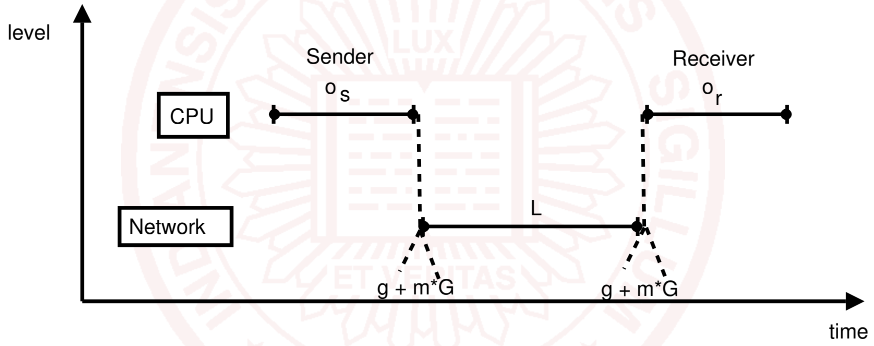
Hardware Parallelism

- More PEs handle more tasks in parallel
- Transistors/PEs take over communication processing
- Communication and computation could run simultaneously

Overlap of Communication and Computation

- Overlap can hide latency
- Improves application performance

The LogGP Model



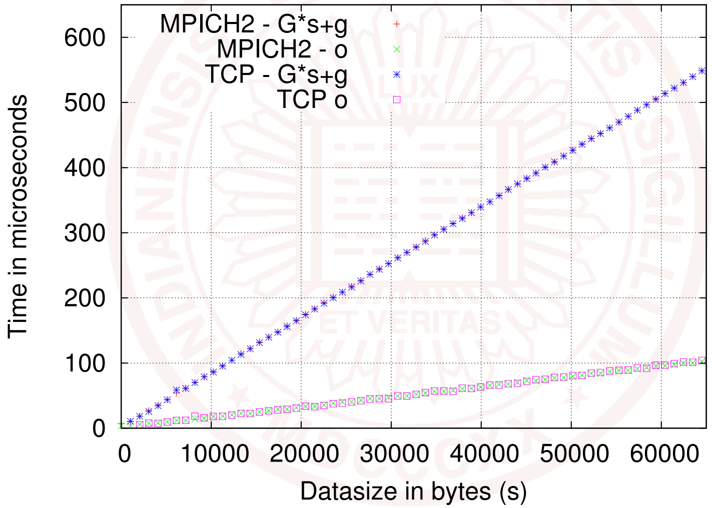
Interconnect Trends

Technology Change

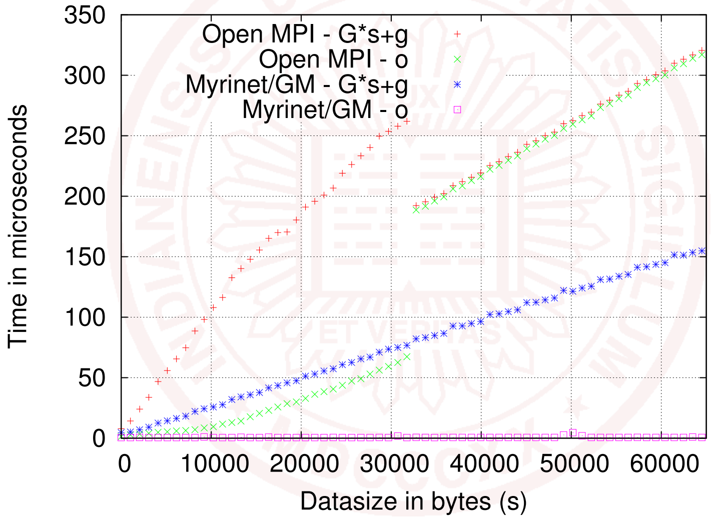
- modern interconnects offload communication to co-processors (Quadrics, InfiniBand, Myrinet)
- TCP/IP is optimized for lower host-overhead (e.g., Gamma)
- even legacy Ethernet supports protocol offload
- $L + g + m \cdot G >> o$

$\Rightarrow$ we prove our expectations with benchmarks of the user CPU overhead

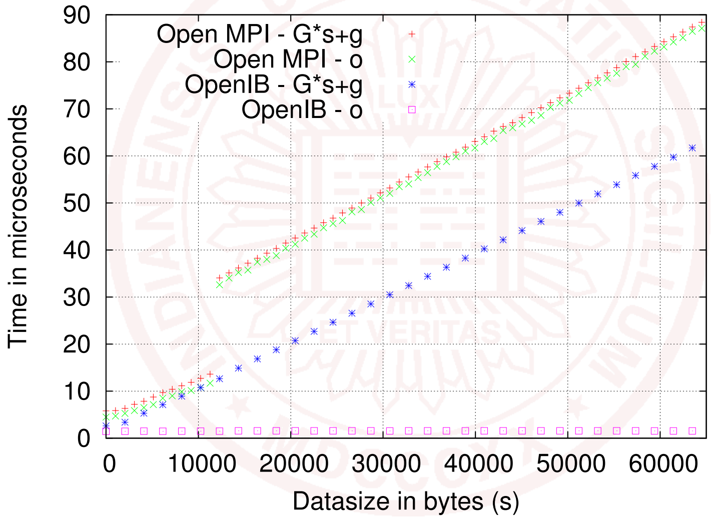
LogGP Model Examples - TCP



LogGP Model Examples - Myrinet/GM



LogGP Model Examples - InfiniBand/OpenIB



Outline

Isend/Irecv is there - Why Collectives?

- Gorlach, ’04: “Send-Receive Considered Harmful”
- $\Leftrightarrow$ Dijkstra, ’68: “Go To Statement Considered Harmful”

point to point

```
if ( rank == 0) then
   call MPI_SEND(...)
else
   call MPI_RECV(...)
end if
```

vs. collective

```
call MPI_GATHER(...)
```

cmp. math libraries vs. loops

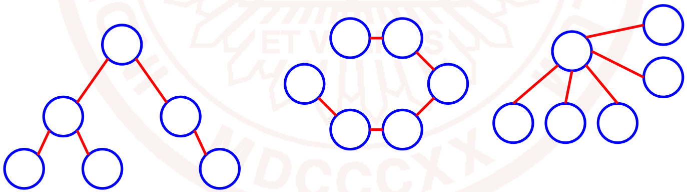
Sparse Collectives

But my algorithm only needs nearest neighbor communication!?
$\Rightarrow$ this is a collective too, just sparse (cf. sparse BLAS)

- sparse communication with neighbors on process topologies
- graph topology makes it generic
- many optimization possibilities (process placing, overlap, message scheduling/forwarding)
- easy to implement
- not part of MPI but fully implemented in LibNBC and proposed to the MPI Forum

Why non blocking Collectives

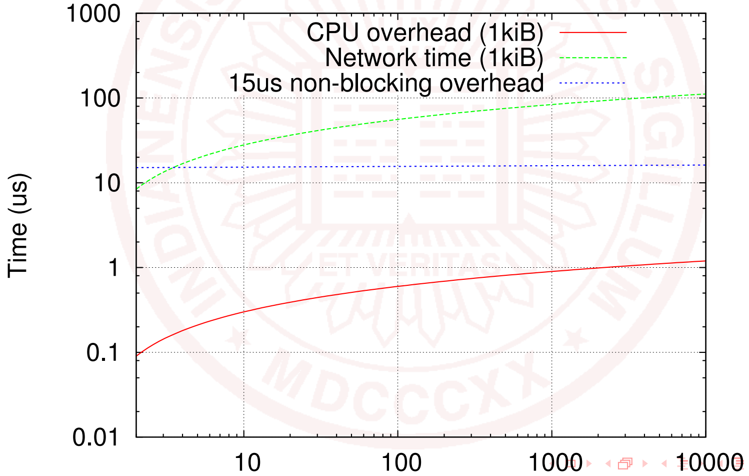
- scale typically with $O(log_2 P)$ sends
- wasted CPU time: $log_2 P \cdot (L + G_{all})$
  - Fast Ethernet: L = 50-60
  - Gigabit Ethernet: L = 15-20
  - InfiniBand: L = 2-7
  - $1 \mu s \approx$ 6000 FLOP on a 3GHz Machine
- ... and many collectives synchronize unneccessarily



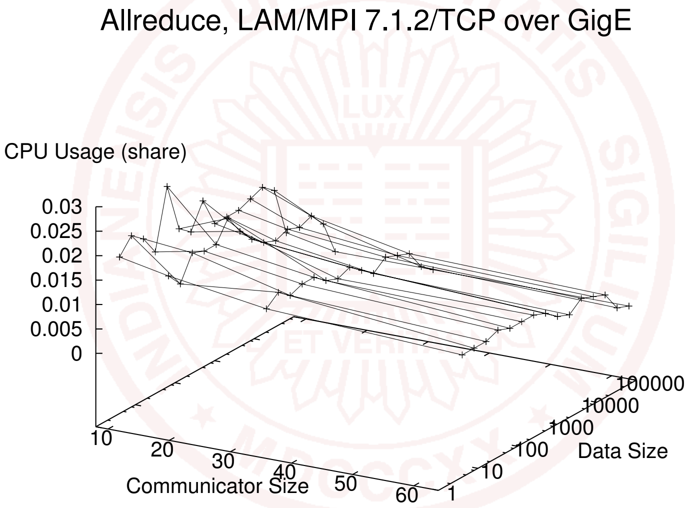
Modelling the Benefits

LogGP Model for Allreduce:

$$t_{allred} = 2 \cdot (2o + L + m \cdot G) \cdot \lceil log_2 P \rceil + m \cdot \gamma \cdot \lceil log_2 P$$



CPU Overhead Benchmarks



Performance Benefits

overlap

- leverage hardware parallelism (e.g. InfiniBand$^{\text{TM}}$)
- overlap similar to non-blocking point-to-point

pseudo synchronization

- avoidance of explicit pseudo synchronization
- limit the influence of OS noise

Process Skew

- caused by OS interference or unbalanced application
- worse if processors are overloaded
- multiplies on big systems
- can cause dramatic performance decrease
- all nodes wait for the last

Example

Petrini et. al. (2003) *”The Case of the Missing Supercomputer Performance: Achieving Optimal Performance on the 8,192 Processors of ASCI Q”*

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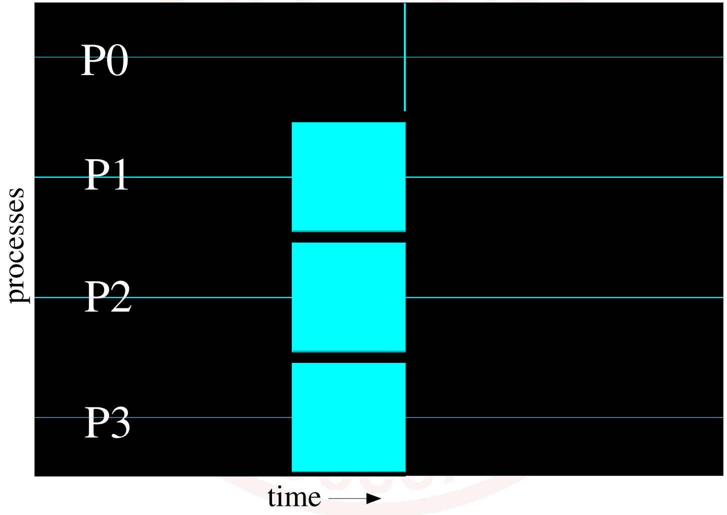
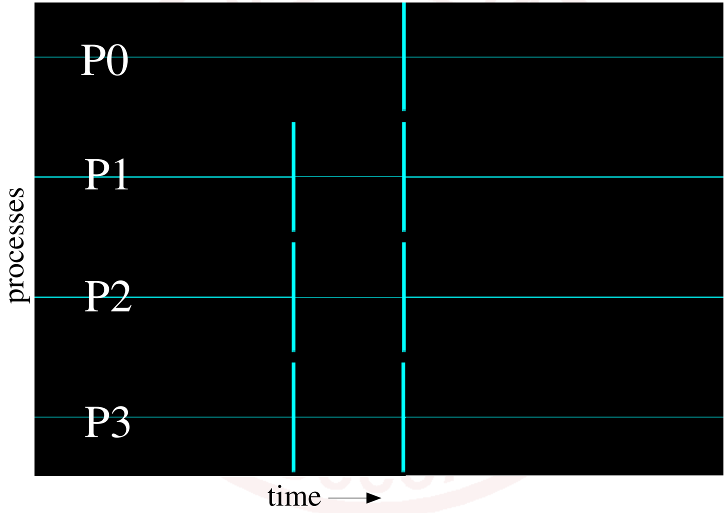
MPI_Bcast with P0 delayed - Jumpshot



MPI_Ibcast with P0 delayed + overlap - Jumpshot



Outline

Non-Blocking Collectives - Interface

- extension to MPI-2
- ”mixture” between non-blocking ptp and collectives
- uses MPI_Requests and MPI_Test/MPI_Wait

Interface

```
MPI_Ibcast(buf, count, MPI_INT, 0, comm, &req);
MPI_Wait(&req);
```

Proposal

Hoefler et. al. (2006): *”Non-Blocking Collective Operations for MPI-2”*

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Non-Blocking Collectives - Implementation

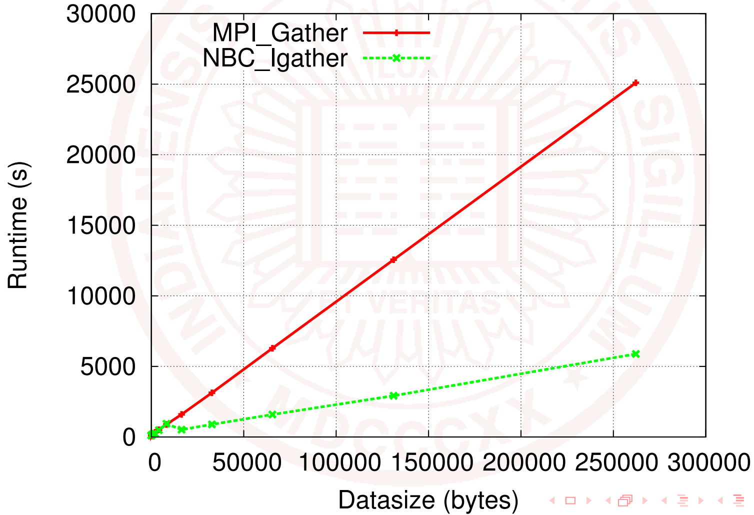
- implementation available with LibNBC
- written in ANSI-C and uses only MPI-1
- central element: collective schedule
- a coll-algorithm can be represented as a schedule
- trivial addition of new algorithms

Example: dissemination barrier, 4 nodes, node 0:

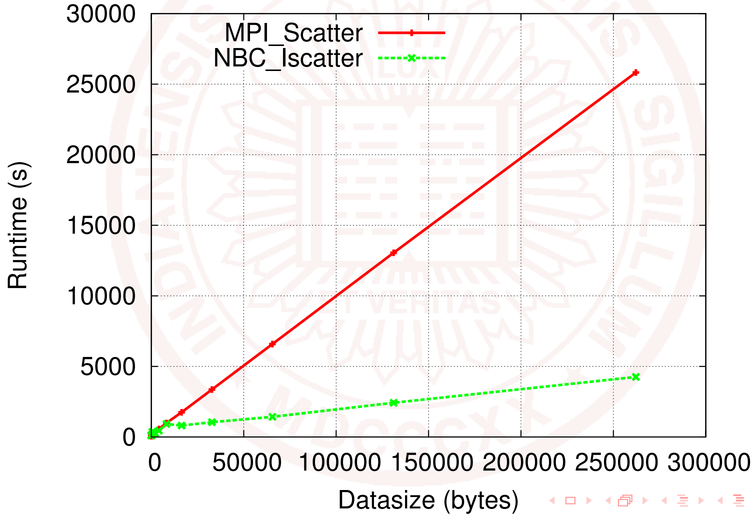
send to 1	recv from 3	end	send to 2	recv from 2	end

LibNBC download: `http://www.unixer.de/NBC`

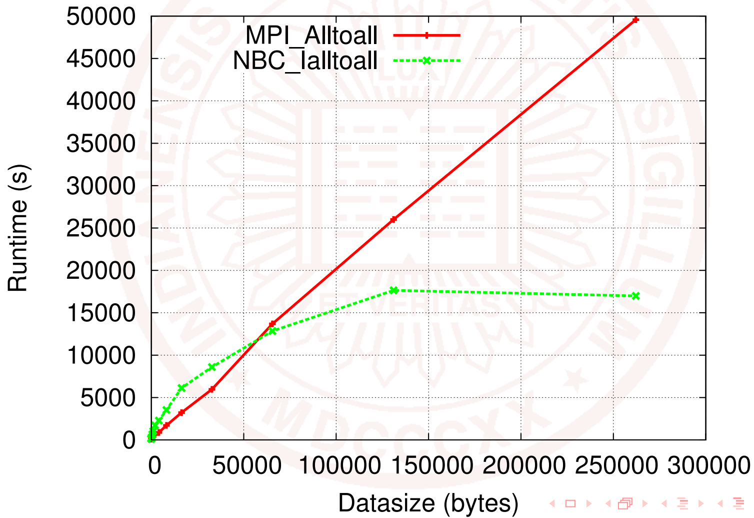
Overhead Benchmarks - Gather with InfiniBand/MVAPICH on 64 nodes



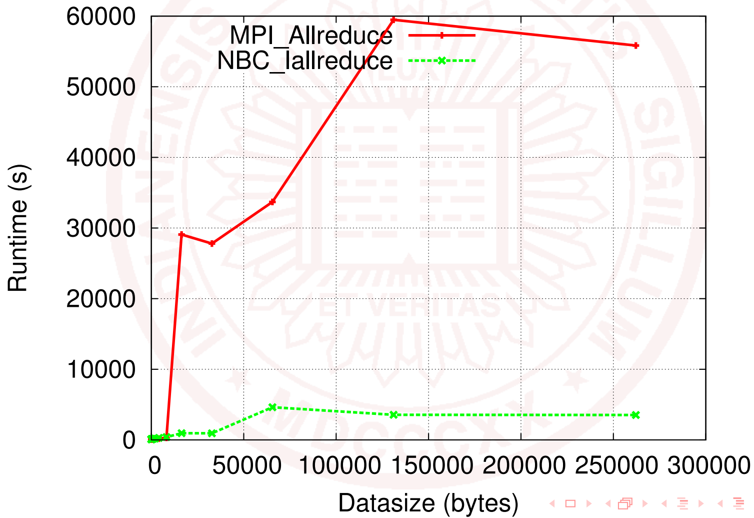
Overhead Benchmarks - Scatter with InfiniBand/MVAPICH on 64 nodes



Overhead Benchmarks - Alltoall with InfiniBand/MVAPICH on 64 nodes



Overhead Benchmarks - Allreduce with InfiniBand/MVAPICH on 64 nodes



Outline

Linear Solvers - Domain Decomposition

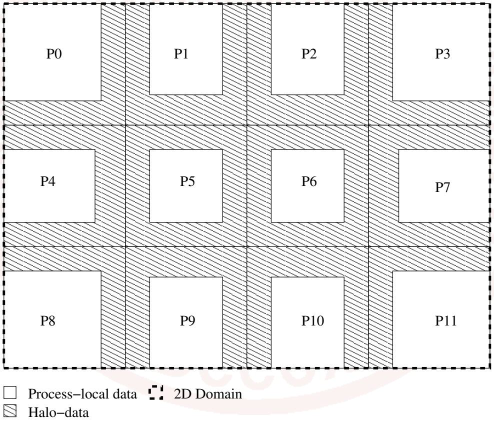
First Example

Naturally Independent Computation - 3D Poisson Solver

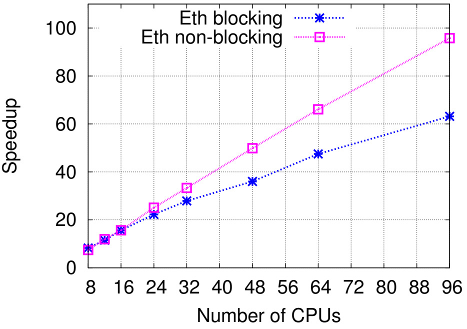
- iterative linear solvers are used in many scientific kernels
- often used operation is vector-matrix-multiply
- matrix is domain-decomposed (e.g., 3D)
- only outer (border) elements need to be communicated
- can be overlapped

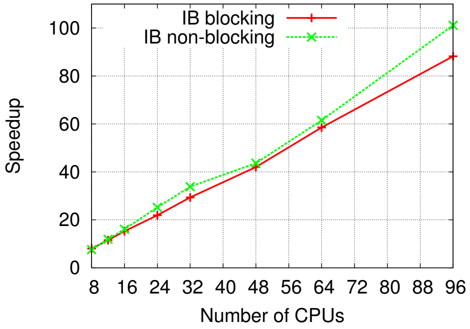
Domain Decomposition

- nearest neighbor communication
- can be implemented with MPI_Alltoallv or sparse collectives



Parallel Speedup (Best Case)





- Cluster: 128 2 GHz Opteron 246 nodes
- Interconnect: Gigabit Ethernet, InfiniBand^{TM}
- System size 800x800x800 (1 node $\approx$ 5300s)

Parallel Data Compression

Second Example

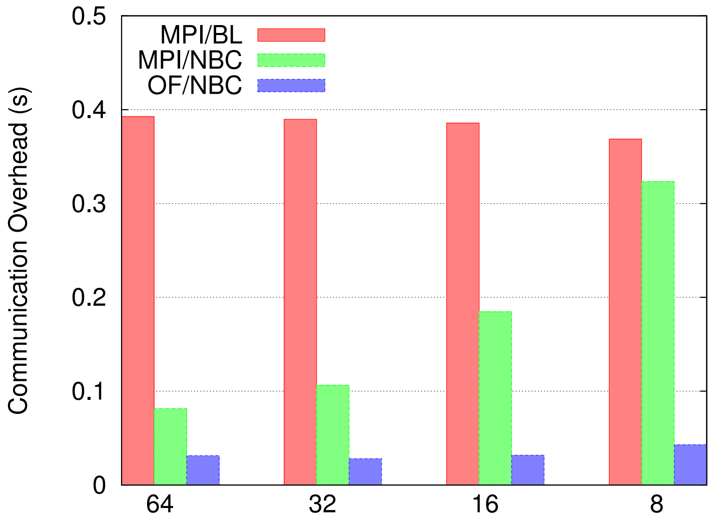
Data Parallel Loops - Parallel Compression

Automatic transformations (C++ templates)

typical loop structure:

```
for (i=0; i < N/P; i++) {
  compute(i);
}
comm(N/P);
```

Parallel Compression Communication Overhead



Parallel 3d Fast Fourier Transform

Third Example

Specialized Algorithms - A parallel 3d-FFT with overlap

Specialized design to achieve the highest overlap. Less cache-friendly!

Non-blocking Collectives - 3D-FFT

Derivation from “normal” implementation

- distribution identical to “normal” 3D-FFT
- first FFT in z direction and index-swap identical

Design Goals to Minimize Communication Overhead

- start communication as early as possible
- achieve maximum overlap time

Solution

- start MPI_Ialltoall as soon as first xz-plane is ready
- calculate next xz-plane
- start next communication accordingly ...
- collect multiple xz-planes (tile factor)

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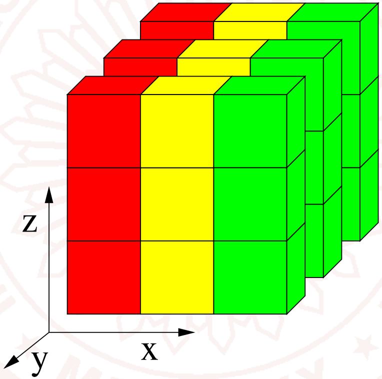
Transformation in z Direction

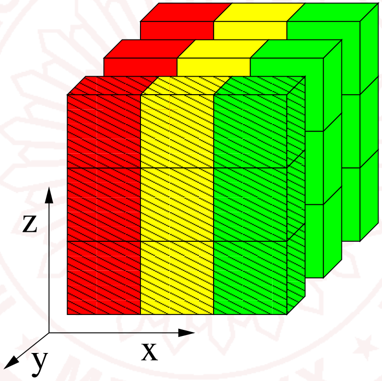
Data already transformed in y direction



1 block = 1 double value (3x3x3 grid)

Transformation in z Direction

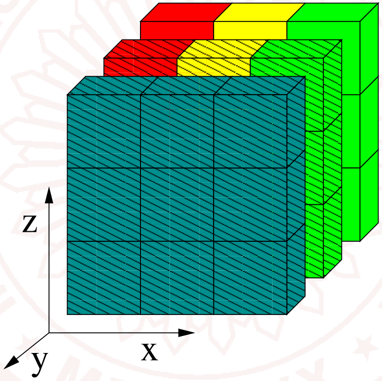
Transform first xz plane in z direction



pattern means that data was transformed in y and z direction

Transformation z Direction

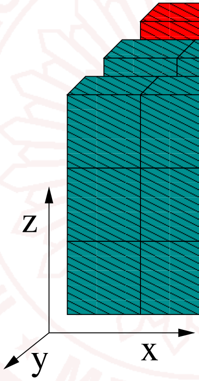
start MPI_Ialltoall of first xz plane and transform second plane



cyan color means that data is communicated in the background

Transformation in z Direction

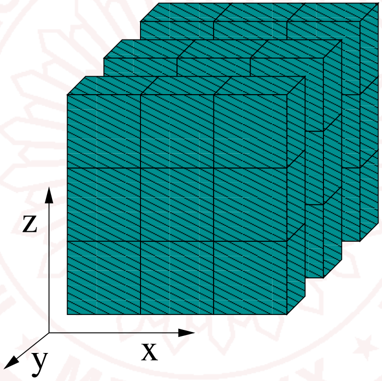
start MPI_Ialltoall of second xz plane and transform third plane



data of two planes is not accessible due to communication

Transformation in x Direction

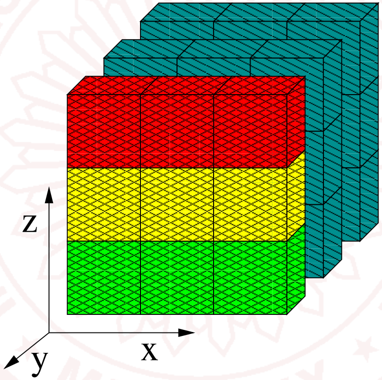
start communication of the third plane and ...



we need the first xz plane to go on ...

Transformation in x Direction

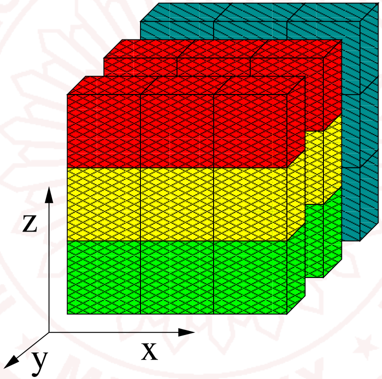
... so MPI_Wait for the first MPI_Ialltoall!



and transform first plane (new pattern means xyz transformed)

Transformation in x Direction

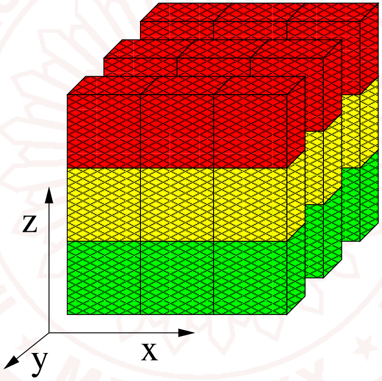
Wait and transform second xz plane



first plane's data could be accessed for next operation

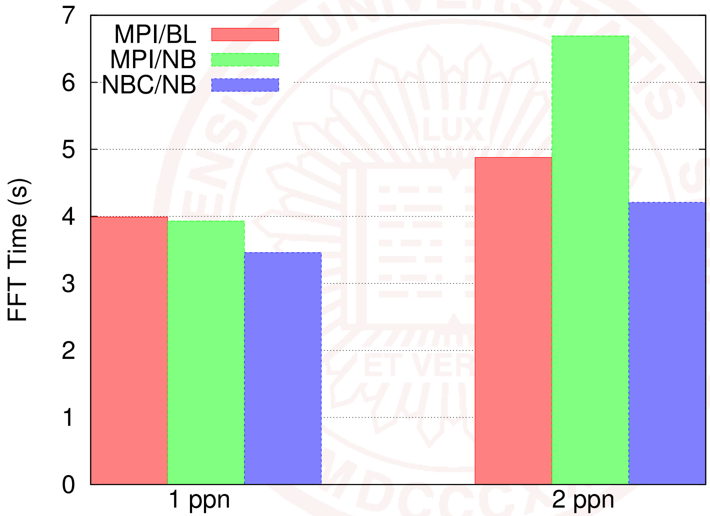
Transformation in x Direction

wait and transform last xz plane



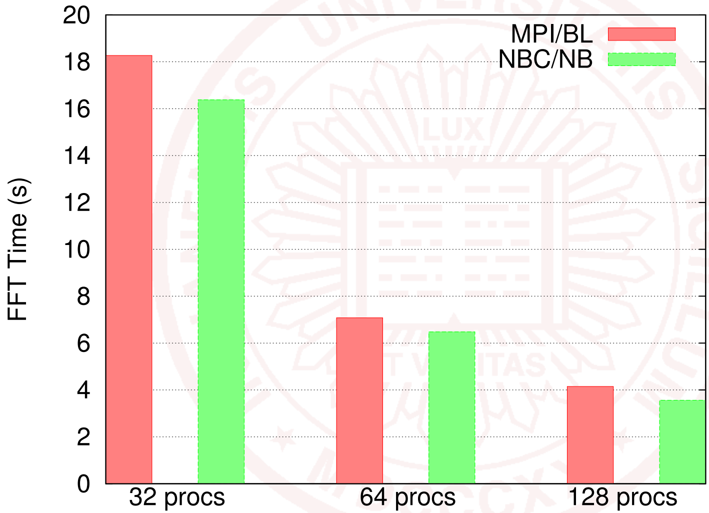
done! → 1 complete 1D-FFT overlaps a communication

1024^3 3d-FFT over InfiniBand



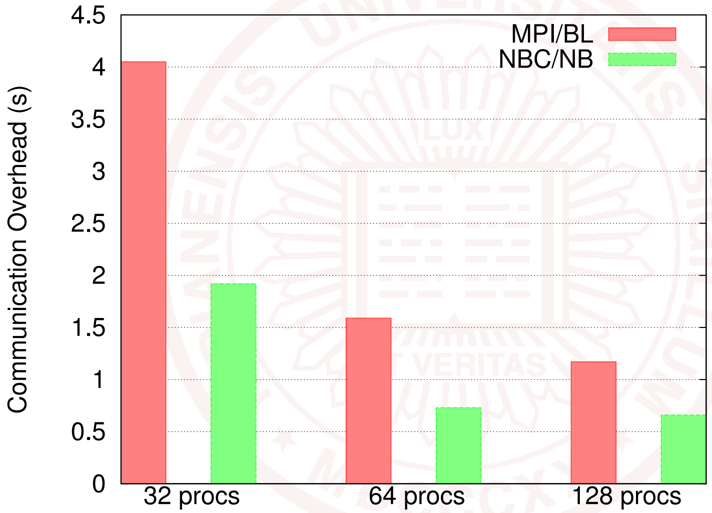
- P=128, "Coyote"@LANL - 128/64 dual socket 2.6GHz Opteron node

1024^3 3d-FFT on the XT4



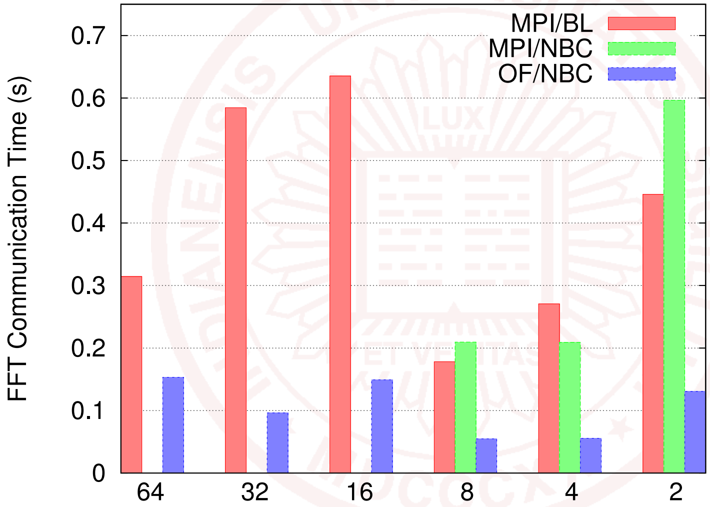
- “Jaguar”@ORNL - Cray XT4, dual socket dual core 2.6GHz Opteron

1024^3 3d-FFT on the XT4 (Communication Overhead)



- "Jaguar"@ORNL - Cray XT4, dual socket dual core 2.6GHz Opteron

640^3 3d-FFT InfiniBand (Communication Overhead)



- “Odin”@IU - dual socket dual core 2.0GHz Opteron InfiniBand

Outline

Ongoing Work

LibNBC

- analysis of multi-threaded implementation
- optimized collectives

Collective Communication

- optimized collectives for InfiniBand^{TM} (topology-aware)
- using special hardware support

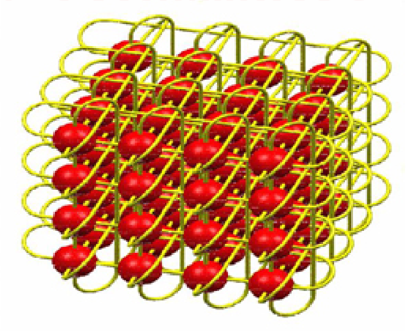
Applications

- work on more applications
- $\Rightarrow$ interested in collaborations (ask me!)

Discussion

THE END

Questions?



Thank you for your attention!