Optimization of a parallel 3d-FFT with non-blocking collective operations

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3rd International ABINIT Developer Workshop
Liège, Belgium
29th January 2007

1. Introduction
   - Short introduction to non-blocking collectives
2. Three dimensional FFTs
   - Traditional parallel 3d-FFT
   - Parallel 3d-FFT with maximum overlap
   - Parallel cache optimized 3d-FFT with partial overlap
3. Implementation in ABINIT
   - Avoidance of the transformation of zeroes
   - Autotuning of parameters
   - Preliminary Performance Results

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Non-blocking Collective Operations

Advantages - Overlap

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

Usage?

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

```
MPI_Ibcast(buf1, p, MPI_INT, 0, comm, &req);
MPI_Wait(&req);
```

Availability

Prototype LibNBC: requires ANSI-C and MPI-2

`LibNBC dowload and documentation:`
`http://www.unixer.de/NBC`

Documentation

T. Hoefler, J. Squyres, W. Rehm, and A. Lumsdaine: *A Case for Non-Blocking Collective Operations*. *In Frontiers of High Performance Computing and Networking, pages 155-164, Springer Berlin, ISBN: 978-3-540-49860-5 Dec. 2006*

T. Hoefler, J. Squyres, G. Bosilca, G. Fagg, A. Lumsdaine, and W. Rehm: *Non-Blocking Collective Operations for MPI-2*. *Open Systems Lab, Indiana University. presented in Bloomington, IN, USA, Aug. 2006*

Performance Benefits?

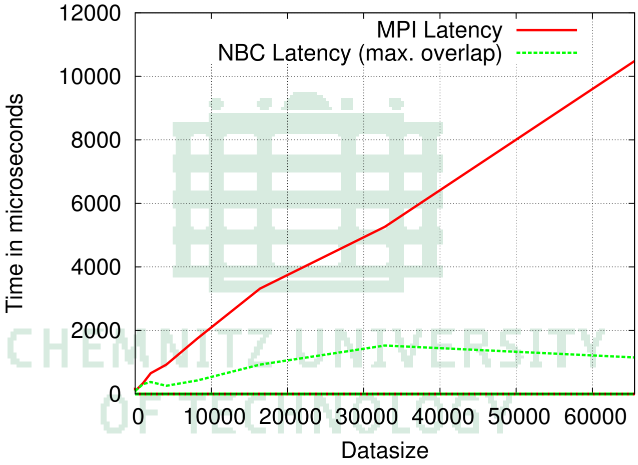
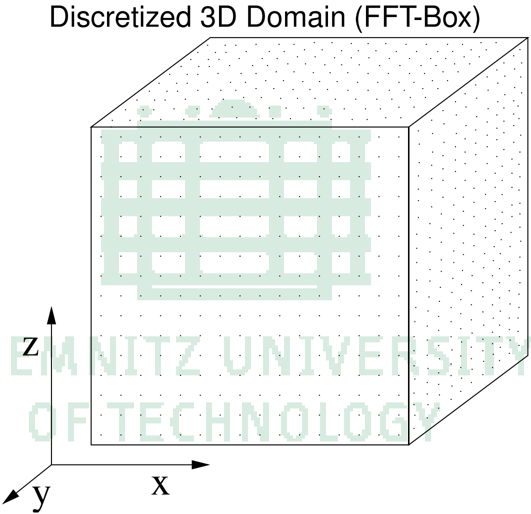
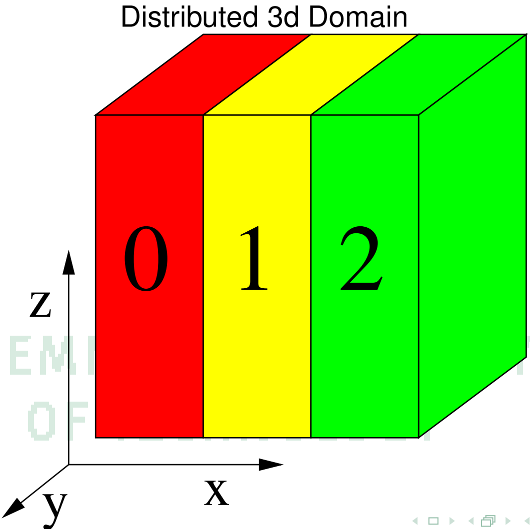


Figure: MPI_Alltoall latency on the “tantale” cluster@CEA

Domain Decomposition

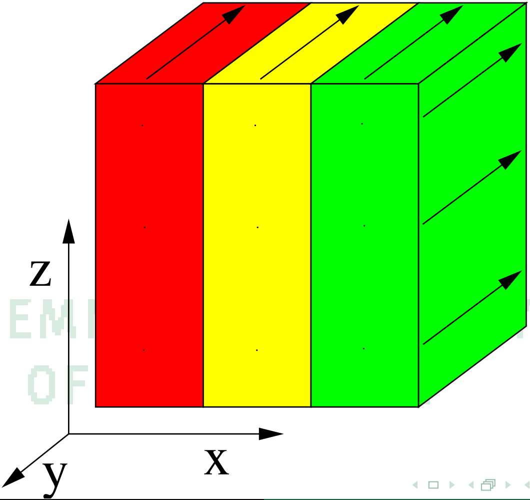


Domain Decomposition



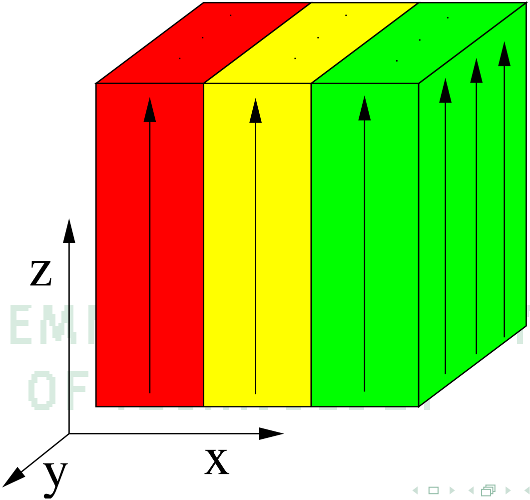
1D Transformation

1D Transformation in y Direction

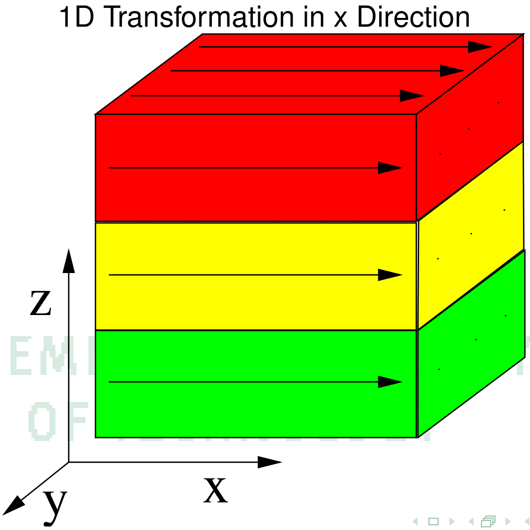


1D Transformation

1D Transformation in z Direction



1D Transformation



Non-blocking 3D-FFT

Derivation from “normal” implementation

- distribution identical to “normal” 3D-FFT
- first FFT in y direction and local data transpose

Design Goals to Minimize Communication Overhead

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

Solution

- start NBC_Ialltoall as soon as first xz-plane is ready
- calculate next xz-plane
- start next communication accordingly ...
- collect multiple xz-planes (A2A data size)

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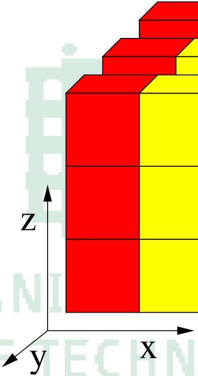
Transformation of in z Direction

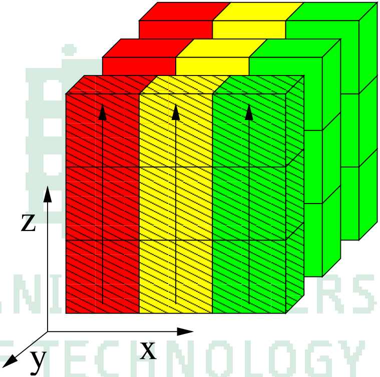
Data already transformed in y direction



1 block = 1 double value (3x3x3 grid)

Transformation of in z Direction

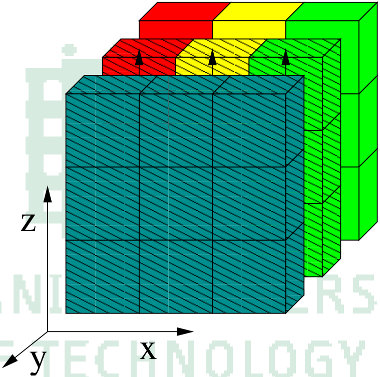
Transform first xz plane in z direction in parallel



pattern means that data was transformed in y and z direction

Transformation of in z Direction

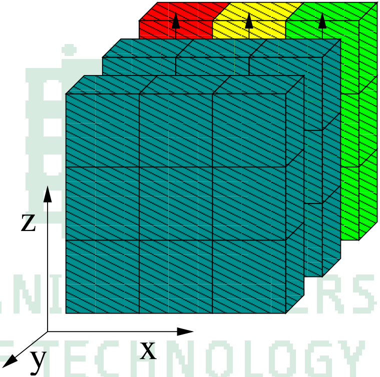
start NBC_Ialltoall of first xz plane and transform second plane



cyan color means that data is communicated in the background

Transformation of in z Direction

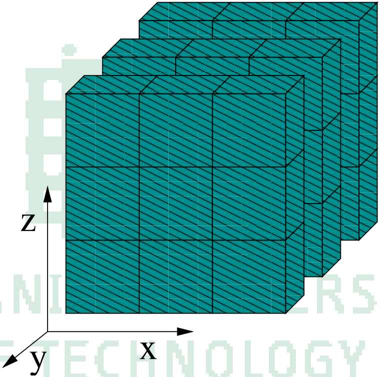
start NBC_Ialltoall of second xz plane and transform third plane



data of two planes is not accessible due to communication

Transformation of in z Direction

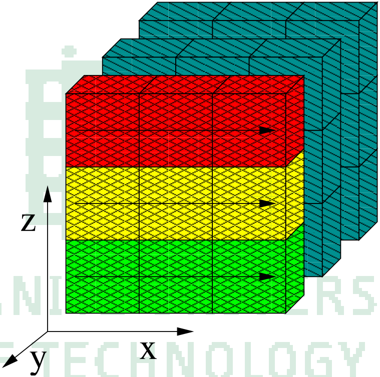
start communication of the third plane and ...



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

Transformation of in x Direction

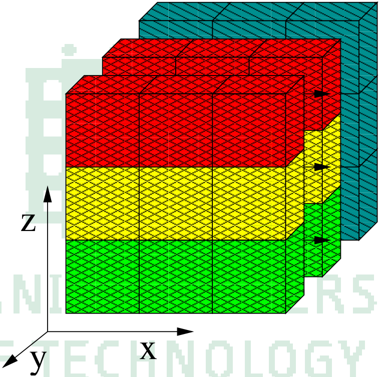
... so NBC_Wait for the first NBC_Ialltoall!



and transform first plane (pattern means xyz transformed)

Transformation of in x Direction

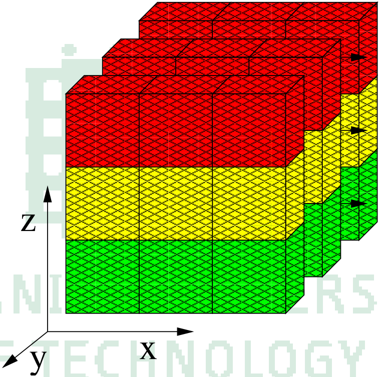
Wait and transform second xz plane



first plane's data could be accessed

Transformation of in x Direction

wait and transform last xz plane



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

Parameter and Problems

Tile factor

- # of z-planes to gather before NBC_Ialltoall is started
- very performance critical!
- not easily predictable

Window size and MPI_Test interval

- Window size = number of outstanding communications
- not very performance critical $\rightarrow$ fine-tuning
- MPI_Test progresses internal state of MPI
- unneccessary in threaded NBC implementation (future)

Problems?

- **NOT** cache friendly :-(

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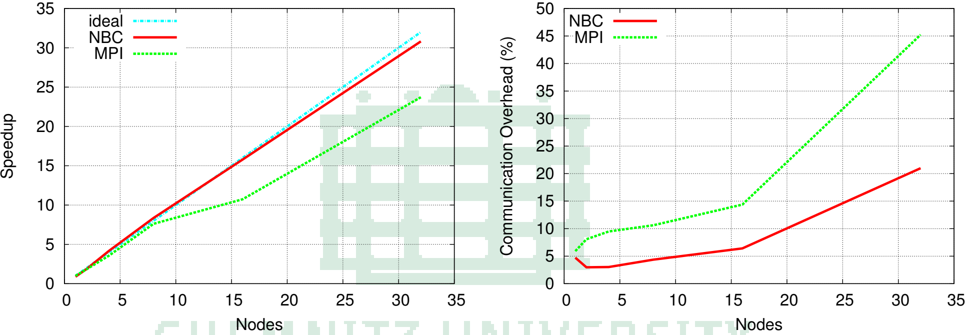
3D-FFT Benchmark Results (small input)



- "tantale"@CEA: 128 2 GHz Quad Opteron 844 nodes
- Interconnect: InfiniBand™
- System size 128x128x128 (1 CPU ≈ 0.75 s)

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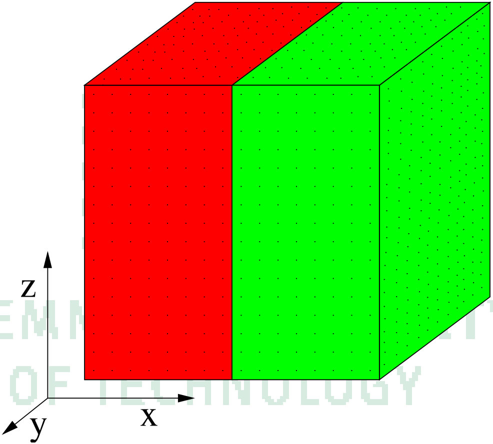
Cache optimal implementation

cache optimality by yz transforming plane by plane (in cache)!



→ we need all yz-planes before we can start x transform :-(

Applying Non-blocking collectives

Pipelined communication

- retain plane-by-plane transform
- simple pipelined scheme
- start A2A of plane as soon as it is transformed
- wait for all before x transform
- A2A overlapped with computation of remaining planes
- last A2A blocks (immediate wait :-( )

Issues

- less overap potential
- plane coalescing to adjust datasize
- new parameter: “pipeline depth” (# of A2As)

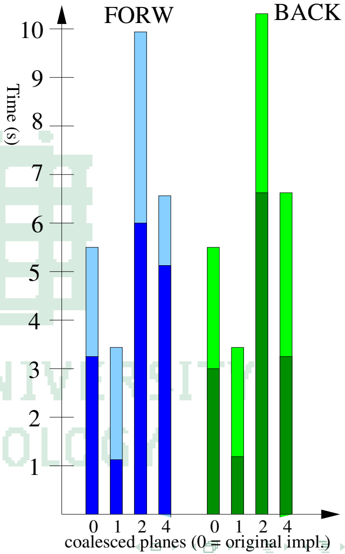
3D-FFT Benchmark Results (small input)

System

- "tantale"@CEA
- 2 GHz Quad Opteron
- InfiniBand™

Parameters

- 128x128x128
- 16 CPUs, 4 nodes
- 1 CPU ≈ 28 s
- 8 planes/proc
- 16kb/plane



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Avoidance of the transformation of zeroes

ABINIT Implementation

- changed routines `back`, `forw`, `back_wf` and `forw_wf`
- some minor changes to others (input params ...)

The routines `back_wf` and `forw_wf`

- avoid transformation of zeroes
- less computation and less communication
- changed communication (boxcut=2):
  - forw_wf: nz/p planes, each has $nx/2 \cdot ny/(2 \cdot p)$ doubles
  - back_wf: $nz/(2 \cdot p)$ planes, each has $nx/2 \cdot ny/p$ doubles

New Parameters

- all routines have different # planes → three parameters

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Autotuning of parameters

Three new input parameters

- `fftplanes_fourdp`, `fftplanes_forw_wf`, and `fftplanes_back_wf`
- default = 0 → standard MPI implementation
- performance critical
- complicated to determine by hand

Autotuning

- automatically determine them at runtime
- each planes parameter is benchmarked (after warmup round)
- fastest is chosen automatically
- relatively accurate but problems with jitter

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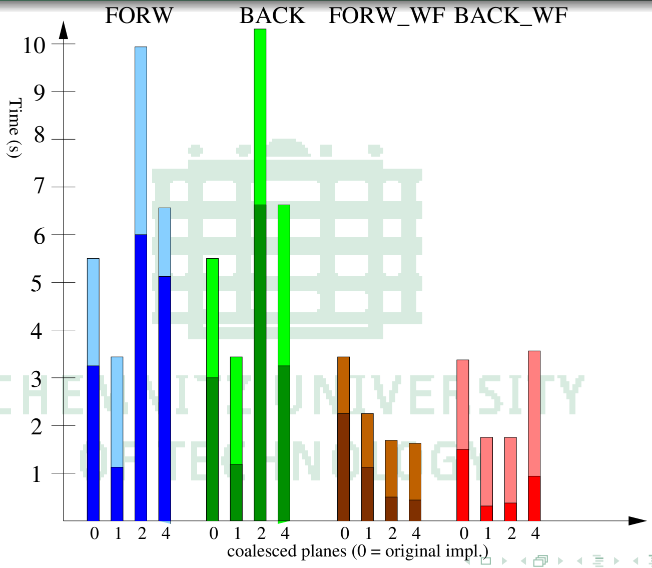
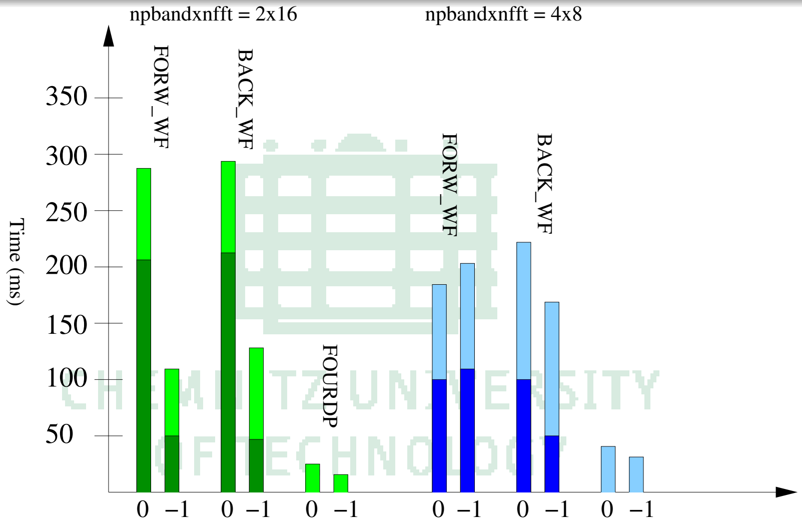
Microbenchmarks



ABINIT - Si, 60 bands, 128^3 FFT



TOTAL 39.5s –> 23.6s 41.1s –> 37.1s

Conclusions & Future Work

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- applying NBC requires some effort
- NBC can improve parallel efficience
- cache usage vs. overlap potential

Future Work

- tune FFT further (reduce serial overhead)
- better automatic parameter assessment (?)
- parallel model for 3d-FFT
- use NBC for parallel orthogonalization
- apply NBC at higher level (LOBPCG?)

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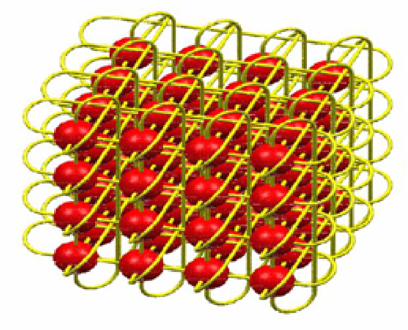
Discussion

ABINIT patch (soon):

`http://www.unixer.de/research/abinit/`



Thanks to the CEA/DAM for support of this work and you for your attention!