Optimised all-to-all communication on multicore architectures applied to FFTs with pencil decomposition

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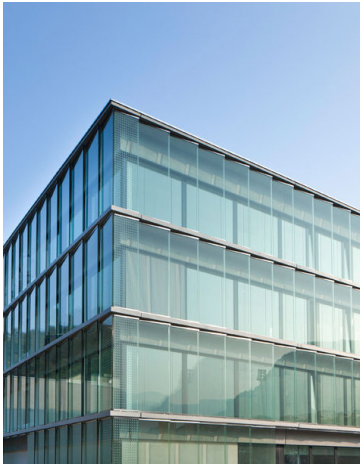


- Basic algorithm
- Generalisation $\rightarrow$ Bruck
- Blocking / non-blocking communication
- GPU-direct
- Applications programming interface
- Benchmarks
- Applications

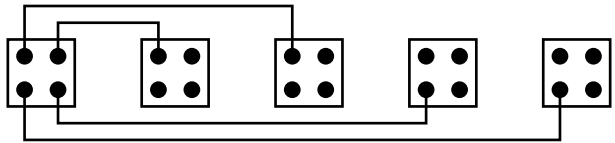
Motivation

- Modern supercomputers equipped with multicore CPUs
- Hybridly — OpenMP + MPI — or pure MPI programmed, focus on MPI only
- If GPUs are present often MPI + CUDA / OpenACC
- Collective communication operations provide fast message transfers for certain communication patterns
- All-to-all personalised communication critical for many applications
- Assumption of a fully connected network, described by latency and bandwidth

Motivation

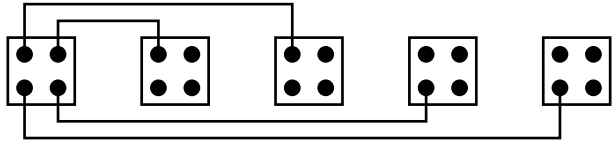
- Scheduling scheme performance critical
- For small messages store and forward algorithms, e.g., Bruck's algorithm
- MPICH, OpenMPI and MVAPICH apply the algorithm with all cores equally connected, the reason should be the current MPI standard
- For allreduce, reduce, broadcast, scatter and gather shared memory parallelism
- Generalised case of multiple all-to-all communication for pencil decomposed FFTs
- Library which exploits shared memory, Li and Laizet CUG 2010
- More efficient communication algorithm for all-to-all / all-to-allv / FFTs introduced here
- "plan" routines, GPU direct supported

Basic all-to-all algorithm



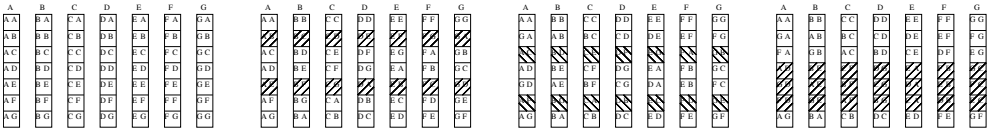
- Communication on the node using shared memory
- Communication between nodes done by multiple (e.g. all) cores

Basic all-to-all algorithm



1. MPI_Irecv
2. memcpy sendbuffer to shared sendbuffer
3. node_barrier
4. MPI_Isend
5. memcpy shared sendbuffer to shared receivebuffer, for data which remains on the node
6. node_barrier
7. MPI_Waitall
8. memcpy shared receivebuffer to receivebuffer

Generalisation → Bruck's algorithm



(a) Initial data

(b) After local rotation

(c) After substep 1 of communication step 1

(d) After substep 2 of communication step 1

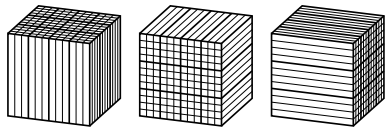
(e) After substep 1 of communication step 2

(f) After substep 2 of communication step 2

(g) After local inverse rotation

- Bruck et al. 1997

Multiple all-to-all algorithm



- For FFTs with pencil decomposition tasks communicate in multiple groups independent from each other
- Our routine includes this case

Blocking communication

- Communication algorithm message size dependent
- Very small messages forwarded between nodes
- Small messages sent directly using the shared memory segment
- Large messages are sent with the original MPI implementation
- Cyclic scheduling is applied
- Throtteling is applied as done in the MPICH reference implementation

Blocking communication

- A “plan” routine is used and a code generator encodes the algorithm
- The execution routine decodes the data
- MPI_Isend, MPI_Irecv, MPI_Wait are used
- Enrichment of the set of opcodes possible
- All-to-allv is implemented without any performance penalty

Non-blocking communication

- For overlapping of communication and computation as done for FFTs
- For no message forwarding and no throtteling one MPI_Waitall present
- Split of the execution in two parts, before and after the waitall, for start and end of the communication

GPU-direct

- Multiple MPI tasks might use one GPU
- Two implementations: small message copied between GPU and CPU and forwarded between nodes
- Large messages are bundled on the GPU with “interprocess communication”
- CUDA kernel which copies from many sourche buffers to many destination buffers

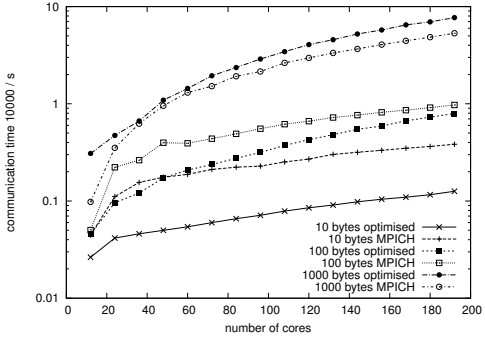
Application programming interface

- Routines are written in ANSI C with different interfaces
- Native one which calles our algorithm with all its parameters
- Automatic one which choses the algorithm and its parameters
- Both options are available in C and Fortran

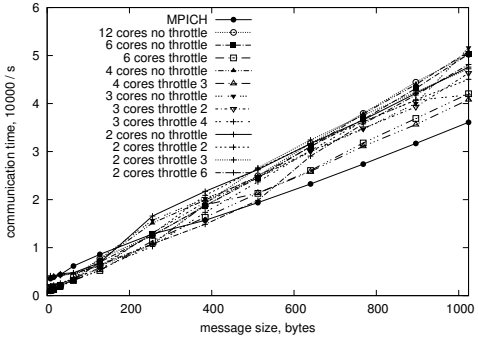
C/C++ : C native interface

```
int EXT_MPI_Alltoall_init_native (void *sendbuf, int sendcount,
    MPI_Datatype sendtype, void *recvbuf, int recvcount, MPI_Datatype
    recvtype, MPI_Comm comm_row, int cores_per_node_row, MPI_Comm
    comm_column, int cores_per_node_column, int num_ports, int
    num_active_ports, int chunks_throttle);
int EXT_MPI_Alltoall_exec_native (int handle);
int EXT_MPI_Alltoall_done_native (int handle);
```

Benchmarks



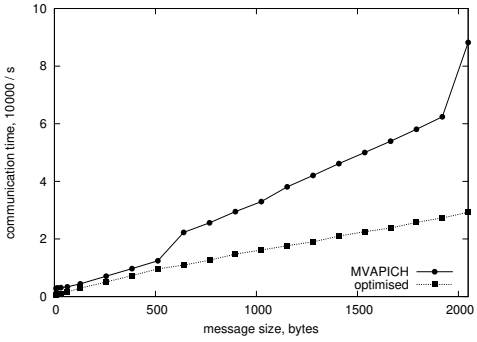
standard all-to-all, 12 nodes, 12 cores per node



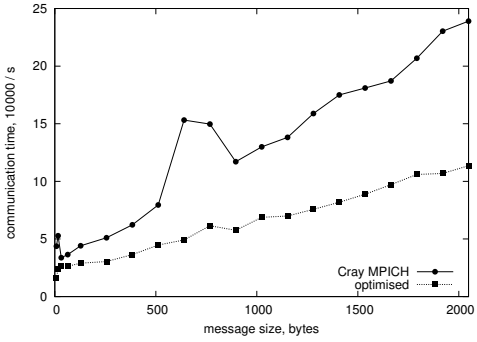
standard all-to-all, variable tile size, 12 nodes, 12 cores per node

- Cray XC50, 12 CPU cores per node, 1 NVIDIA Tesla P100
- Cray XC 40 KNL, 12 cores used per KNL

Benchmarks



all-to-all on Piz Kesch, 5 nodes, 12 cores per node

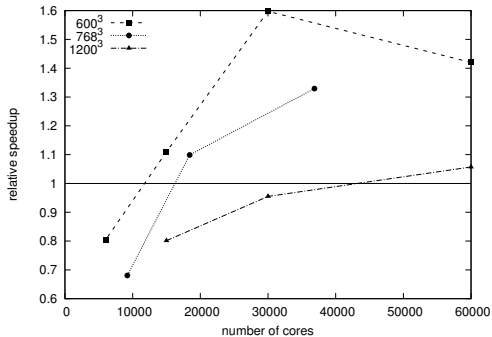


GPU-direct, 12 nodes, 12 cores per node

- Infiniband cluster Piz Kesch (Meteoswiss)
- GPU-direct on Piz Daint

Applications: LATfield2

- Spectral code with real-to-complex 3D FFTs and complex-to-real 3D FFTs
- High memory requirement $\rightarrow$ small messages originating from FFTs



relative speedup for FFTs

Applications: ORB5

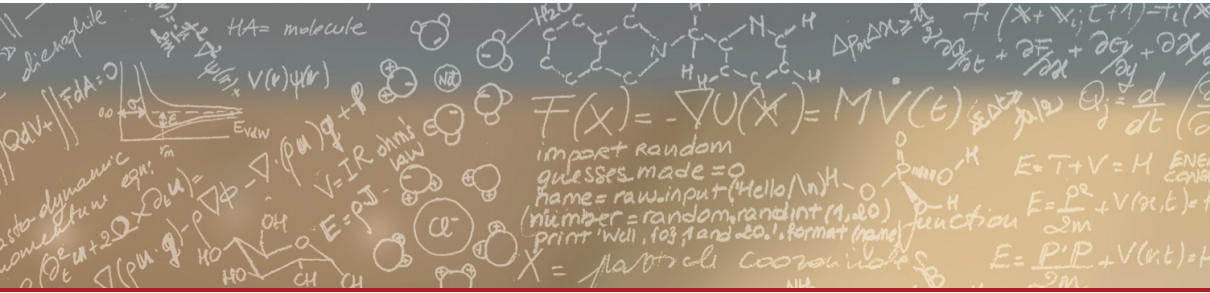
- Particle in cell code with toroidal domain
- MPI parallelisation in subdomains and clones
- Random variable message sizes for particle exchange between all subdomains (all-to-all communication)
- Typically all clones of a specific subdomain on a node $\rightarrow$ application for our algorithm

Discussion

- Implementation of the single all-to-all algorithm in the current MPI standard possible but would slowdown the communicator creation
- Multiple all-to-all possible with a graph communicator, also computationally expensive
- Suggestion: extension of the MPI standard with ”plan” routines

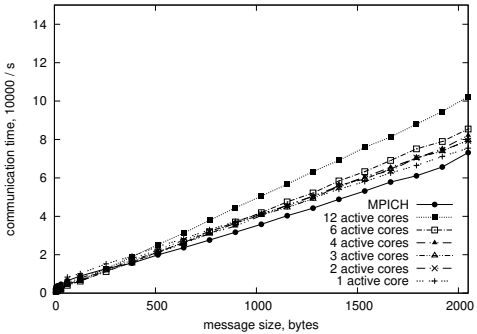
Conclusions

- Message passing algorithm for all-to-all communication for networks with shared memory nodes
- Cray MPICH outperformed by a factor of 2.9 for 10 bytes messages
- On infiniband cluster standard MVAPICH outperformed for small messages
- GPU implemenation advantegous for small and medium message size
- Application to FFTs (LATfield2) demonstrates its strength

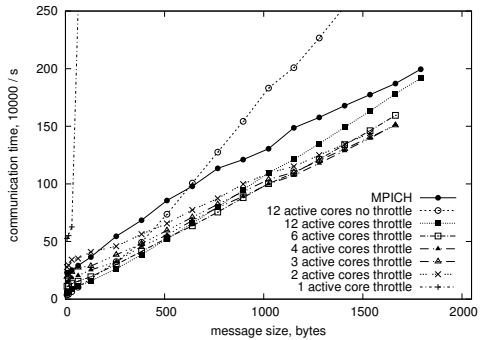


Thank you for your attention.

Benchmarks

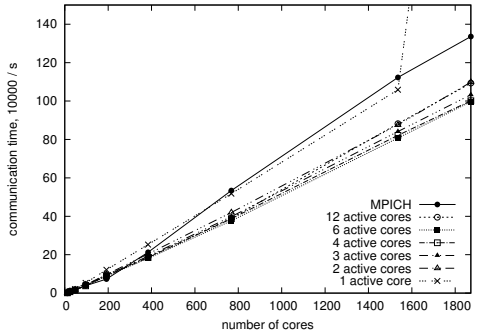


standard all-to-all, variation of active number of cores, 12 nodes, 12 cores per node



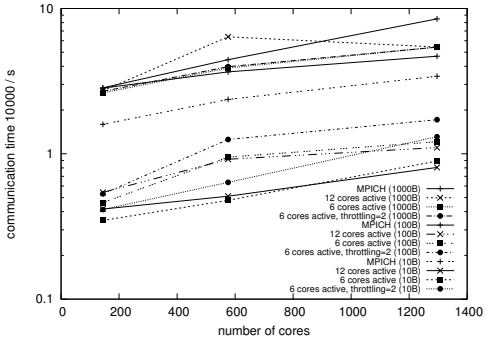
standard all-to-all, 156 nodes, 12 cores per node

Benchmarks

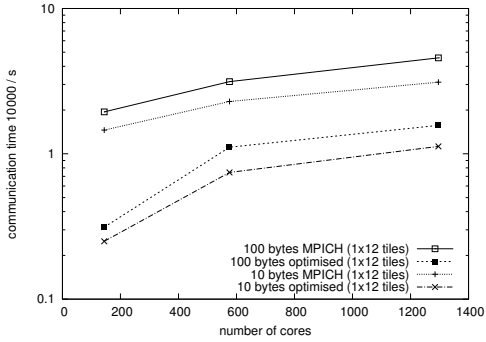


standard all-to-all, 1024 bytes, 12 cores per node, throttle

Benchmarks



multiple all-to-all 3 × 4 cores



multiple all-to-all 1 × 12 cores