

## pMR: A high-performance communication library\*

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On many parallel machines, the time LQCD applications spent in communication is a significant contribution to the total wall-clock time, especially in the strong-scaling limit. We present a novel high-performance communication library that can be used as a de facto drop-in replacement for MPI in existing software. Its lightweight nature that avoids some of the unnecessary overhead introduced by MPI allows us to improve the communication performance of applications without any algorithmic or complicated implementation changes. As a first real-world benchmark, we make use of the pMR library in the coarse-grid solve of the Regensburg implementation of the DD- $\alpha$ AMG algorithm. On realistic lattices, we see an improvement of a factor 2x in pure communication time and total execution time savings of up to 20%.

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## 1. Introduction and motivation

The Regensburg group (RQCD) has shown that their implementation of the DD- $\alpha$ AMG algorithm [1], targeting the first-generation Intel Xeon Phi architecture (a.k.a. KNC), is well optimized in terms of computation and that its run time is now dominated by off-chip communication [2]. For off-chip communication, our implementation of DD- $\alpha$ AMG uses the Message Passing Interface (MPI). Hence the performance depends on the specific MPI implementation used. We use Intel MPI, which is the de facto choice for applications running natively on the KNC. Unfortunately, its closed-source character does not allow us to directly contribute any improvements. Developing a new MPI-conformant library would involve major efforts and would not be sensible anyway since most parts of MPI are either not required or only used in parts that are not performance-critical. Contributing to an existing open-source MPI implementation is an option, but we would then have to strictly adhere to the MPI standard. Relaxing this constraint allows us to design a new API with performance benefits not possible otherwise. We therefore decided to develop a novel high-performance communication library well suited for DD- $\alpha$ AMG and stencil-type applications in general, with QPACE 2 [3] being the initial target.

## 2. Overview of the communication library

Before designing a new high-performance communication library some key objectives have to be identified. The most obvious is to efficiently utilize all available resources of the network hardware. In the case of QPACE 2, which uses InfiniBand FDR for off-chip communication, this includes using Remote Direct Memory Access (RDMA) capabilities. This is the origin of the name pico Message Passing for RDMA (pMR) [4] of the communication library. Efficient usage of InfiniBand hardware requires re-using hardware resources that have been established once as often as possible. Hence pMR was designed with persistent communication in mind. RDMA and persistent communication help to minimize the latency imposed by the hardware. Any additional software-induced latency should be reduced to a bare minimum. To achieve this goal we adhere to a few coding restrictions, e.g., no polymorphism at all to avoid vtable lookups. In addition, we do not spawn any extra threads within the library to avoid context switches.<sup>1</sup>

As it is not feasible to implement all MPI features and re-write all existing software to use pMR instead of MPI, it should be possible to use both at the same time and to allow porting to pMR piece by piece. To facilitate the latter, the pMR API differs only slightly from MPI so that no major code modifications are required. Furthermore, the simplicity of pMR allows us to adapt to new networking hardware and to support new network topologies with only modest efforts.

For the implementation, we chose C++11 with an optional C API. An important objective when writing the code was to minimize dependencies. E.g., code for each supported network provider is isolated to allow for easy addition or removal without effects on any other provider. Apart from improving maintainability this allows for compile-time optimizations by only enabling required network providers. As a consequence, binaries are cluster specific.

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<sup>1</sup>This is in contrast to many MPI implementations which spawn an arbitrary number of threads to improve performance. However, experience shows that these threads often interact with the application's threads and thus cause context switches and degrade performance. In some MPI implementations these internal threads are not even pinnable.

### 3. Porting existing software to pMR

#### 3.1 General implementation notes

One of the key objectives of pMR is to allow for easy successive porting of existing MPI C++ (and C) software. This process depends on the particular MPI communication method. The only two methods discussed in this section are persistent and non-persistent point-to-point communication. These two methods are probably the most common ones. The difference to pMR for the former is depicted in Fig. 1.<sup>2</sup> In this case, two small modifications are sufficient. First, pMR requires the user to setup persistent connections to maximize the possible re-use of resources. Second, both send and receive routines are split into three functions instead of two to allow for further overlap of communication and computation. In both MPI and pMR, to have persistent send and receive buffers, we need handles associated with a particular buffer. These handles provide all required data to allow for re-using resources for data transfers working on the same buffer. Hence a

```

MPI_Request sendRequest;
MPI_Request recvRequest;

// Setup persistent transfer buffers
MPI_Send_init(sendBuffer, count, MPI_FLOAT,
              target, sendTag, Comm, sendRequest);
MPI_Recv_init(recvBuffer, count, MPI_FLOAT,
              target, recvTag, Comm, recvRequest);

for(i = start; i != end; ++i)
{
    // Computation

    MPI_Start(recvRequest);
    MPI_Start(sendRequest);

    // Computation

    MPI_Wait(sendRequest, MPI_STATUS_IGNORE);
    MPI_Wait(recvRequest, MPI_STATUS_IGNORE);

    // Computation
}

MPI_Request_free(recvRequest);
MPI_Request_free(sendRequest);

// Setup persistent connection
pMR::Connection connection(pMR::Target(
    Comm, target, sendTag, recvTag));

// Setup persistent transfer buffers
pMR::SendWindow<float> sendWindow(
    connection, sendBuffer, count);
pMR::RecvWindow<float> recvWindow(
    connection, recvBuffer, count);

for(i = start; i != end; ++i)
{
    // Computation

    recvWindow.init();
    sendWindow.init();

    // Computation

    sendWindow.post();
    recvWindow.post();

    // Computation

    sendWindow.wait();
    recvWindow.wait();

    // Computation
}

```

**Figure 1:** Halo exchange using persistent MPI point-to-point communication vs. pMR.

<sup>2</sup>Note that the pseudo-code in Figs. 1 and 2 is missing proper error handling. For MPI it is necessary to check the return value of almost all MPI functions for success. pMR is using C++ exception handling, i.e., it throws an exception whenever an error occurs.

```

MPI_Request sendRequest;
MPI_Request recvRequest;

// Setup persistent connection
pMR::Connection connection(pMR::Target(
    Comm, target, sendTag, recvTag));

// Setup persistent transfer buffers
pMR::SendWindow<float> sendWindow(
    connection, sendBuffer, count);
pMR::RecvWindow<float> recvWindow(
    connection, recvBuffer, count);

for(i = start; i != end; ++i)
{
    // Computation

    MPI_Irecv(recvBuffer, count, MPI_FLOAT,
        target, recvTag, Comm, recvRequest);
    MPI_Isend(sendBuffer, count, MPI_FLOAT,
        target, sendTag, Comm, sendRequest);

    // Computation

    MPI_Wait(sendRequest, MPI_STATUS_IGNORE);
    MPI_Wait(recvRequest, MPI_STATUS_IGNORE);

    // Computation
}

// Setup persistent connection
pMR::Connection connection(pMR::Target(
    Comm, target, sendTag, recvTag));

// Setup persistent transfer buffers
pMR::SendWindow<float> sendWindow(
    connection, sendBuffer, count);
pMR::RecvWindow<float> recvWindow(
    connection, recvBuffer, count);

for(i = start; i != end; ++i)
{
    // Computation

    recvWindow.init();
    sendWindow.init();

    // Computation

    sendWindow.post();
    recvWindow.post();

    // Computation

    sendWindow.wait();
    recvWindow.wait();

    // Computation
}

```

**Figure 2:** Halo exchange using non-persistent MPI point-to-point vs. pMR.

data transfer is initiated by the handle instead of the associated buffer. pMR uses different handles for send and receive buffers, i.e., the `SendWindow` and `RecvWindow` classes.

For the case of non-persistent MPI one more step is required when moving to pMR (see Fig. 2): since pMR is persistent, we need to introduce handles for the send and receive buffers as explained above. This step could have the consequence of fundamental code changes since we need to refer to the handles when performing data transfers, i.e., these changes are imposed by the switch from the non-persistent to the persistent communication model. If desired, the changes can be minimized at the cost of introducing some buffering overhead as described below.

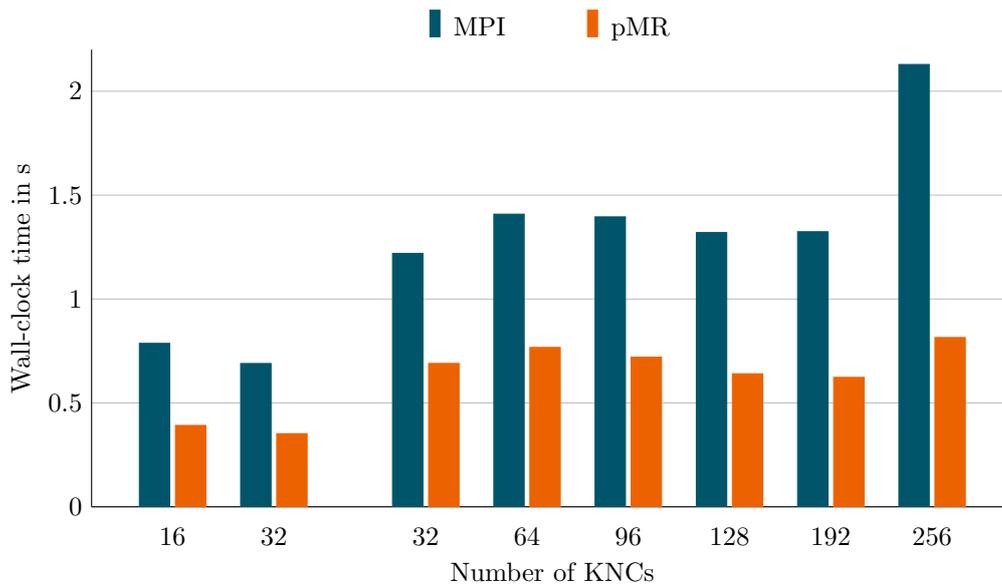
### 3.2 Porting the RQCD DD- $\alpha$ AMG implementation to pMR

We chose the coarse-grid part of the DD- $\alpha$ AMG algorithm as the first real-world benchmark for pMR as it was shown earlier to be communication bound. We use the two-level version, for which the only operation on the coarse-grid is a solve using the FGMRES iterative solver. The only performance-relevant communications in FGMRES are halo exchanges and global sums. For now we only optimized the former, which were previously implemented as non-persistent MPI point-to-point communication. To avoid major code changes due to persistent communication handles, buffering for send and receive data was introduced, i.e., the data to be transferred are first copied to a registered send buffer, and received data are copied from a registered receive buffer to the actual

location. This adds additional overhead, but for this first benchmark we decided to pay this price to keep code changes to a minimum. Incidentally, the coarse-grid solver requires such buffering for half of its data transfers anyway since it reduces the number of packages sent over the network by gather/scatter operations to/from buffers. To minimize this overhead we have first threaded the (previously unthreaded) copy process to/from send/receive buffers. This is especially important on the KNC, where the memory bandwidth scales linearly with the number of active cores. While this also helps to improve the performance for MPI, we do not provide any details on this point. All data shown below are with multi-threaded copy enabled for both MPI and pMR.

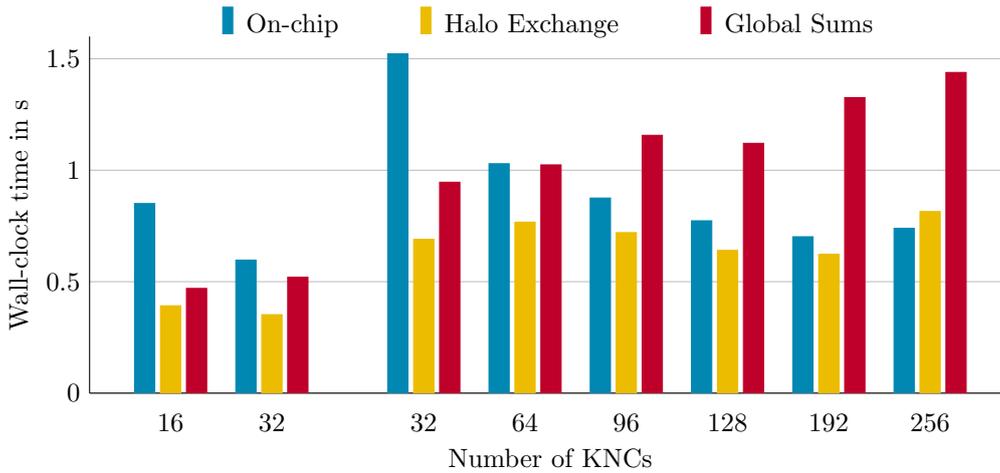
#### 4. Results

The benchmarks were run on QPACE 2 and QPACE B. Both machines use KNC coprocessors and an InfiniBand network; for details see Table 1 and Ref. [3]. Software and Intel MPI details are given in Table 2, while details of the CLS lattices [5] used in the runs are shown in Table 3. For the benchmark runs on QPACE B, the differences in the run times are solely due to the differences between MPI and pMR. For QPACE 2 there is an additional topology effect: QPACE 2 uses a novel topology called Flexible Block Torus, which Intel MPI is not aware of.



**Figure 3:** Time spent in halo exchanges in the coarse-grid part of a single solve. The two left-most pairs of bars are results from QPACE B, while the others are from QPACE 2, with fixed problem size in both cases.

The results in Fig. 3 for the wall-clock time spent in halo exchanges (including copying of data to/from buffers) shows an improvement of about a factor 2x for pMR compared to MPI for both clusters. This is a significant improvement. The increase for 32 to 64 and 192 to 256 KNCs is due to the mapping of the lattice to nodes, see Table 4 for details. In every distributed space-time dimension (i.e., a dimension involving multiple nodes) two messages need to be sent for each halo exchange, i.e., the number of packages required per halo exchange is equal to the number of distributed dimensions times two. For a fixed number of distributed dimensions the time spent in halo exchanges decreases with the number of KNCs as the message size decreases.



**Figure 4:** Contributions to run time spent on the coarse-grid part of a single solve using pMR for halo exchanges. The two left-most groups of bars are results from QPACE B, the others are from QPACE 2, with fixed problem size in both cases.

Figure 4 shows the contribution of the time spent on-chip (computation and on-chip synchronization), halo exchanges, and global sums for the coarse-grid solve, using pMR for halo exchanges only. Due to the improvements obtained from utilizing pMR for halo exchanges, the time spent on-chip is now almost equal to the sum of halo exchanges and global sums for a low number of KNCs. Scaling to a higher number of KNCs at fixed problem size, the global sums become the dominant contribution. Hence, to achieve better strong scaling of the coarse grid part it is crucial to improve (or reduce the number of) global sums. In other words, they are the next target for pMR.

In the case of 256 KNCs there are two interesting observations. First, we see an increase in the on-chip contribution for this particular fixed problem size. The reason is that the local problem size per KNC is too small to efficiently utilize the available resources and the on-chip synchronization overhead is critical. Second, when running with MPI only, the time spent in global sums is about twice larger than when running with pMR for halo exchanges (but not for global sums). We do not have an explanation for the second observation.

## 5. Conclusions and outlook

By replacing MPI with pMR in the halo exchanges of the DD- $\alpha$ AMG coarse-grid solve we were able to significantly reduce the share of total wall-clock time for this previously dominant contribution. We have therefore been able to demonstrate that communication-bound stencil-type applications can be notably improved by utilizing our novel high-performance communication library without major code changes, let alone algorithmic changes.

For the DD- $\alpha$ AMG coarse-grid solve the global sums are now the dominant part. Therefore we plan to extend the preliminary global reductions support of pMR and implement it in the RQCD DD- $\alpha$ AMG implementation. This is especially important to improve the coarse-grid scaling behavior. However, currently the main priority is to add support for our new cluster QPACE 3 to pMR. QPACE 3 is not using InfiniBand for inter-node communication, but Intel Omni-Path, a technology that is very different to InfiniBand in several aspects.

## A. Benchmark details

	Host Xeon	Xeon Phi	InfiniBand	Topology
QPACE 2	E3-1230L v3	4x 7120X	Connect-IB FDR	Flexible Block Torus
QPACE B	E5-2603 v2	2x 31S1P	ConnectX-2 QDR	Single switch

**Table 1:** Hardware overview.

OS	Intel MPSS	OFED	Intel MPI	MPI provider	Allreduce
CentOS 7	3.5.1	3.12-1	5.1 Update 3	DAPL (CCL-direct only)	Recursive doubling

**Table 2:** Software overview.

	id	$\beta$	$N_s$	$N_t$	$m_\pi$	$a$
QPACE 2	C101	3.4	48	96	220 MeV	0.086 fm
QPACE B	H102	3.4	32	96	350 MeV	0.086 fm

**Table 3:** CLS lattice configurations used for benchmarks [5].

16	32	64	96	128	192	256
$1 \times 1 \times 2 \times 8$	$1 \times 1 \times 4 \times 8$	$1 \times 4 \times 4 \times 4$	$1 \times 4 \times 3 \times 8$	$1 \times 4 \times 4 \times 8$	$1 \times 4 \times 4 \times 12$	$2 \times 4 \times 4 \times 8$

**Table 4:** Mapping of the lattice (bottom) to number of KNCs (top). The RQCD DD- $\alpha$ AMG implementation imposes some restrictions on the possible mappings. We picked the mappings that minimize the total execution time for MPI.

## References

- [1] A. Frommer et al., *Adaptive Aggregation Based Domain Decomposition Multigrid for the Lattice Wilson Dirac Operator*, *SIAM J. Sci. Comput.* **36** (2014) A1581 [arXiv:1303.1377].
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