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A fast MPI-based Distributed Hash-Table as Surrogate Model demonstrated in a coupled reactive transport HPC simulation

Max Lübke[1], Marco De Lucia[2], Stefan Petri[3], and Bettina Schnor[1]

[1] University of Potsdam, Institute of Computer Science, An der Bahn 2, 14476 Potsdam, Germany
{mluebke,schnor}@uni-potsdam.de
[2] GFZ Helmholtz Centre for Geosciences, Telegrafenberg, 14473 Potsdam, Germany
delucia@gfz.de
[3] Potsdam Institute for Climate Impact Research, Member of the Leibniz Association, Telegrafenberg, 14473 Potsdam, Germany
petri@pik-potsdam.de

Abstract. This is an extended version of the paper "A fast MPI-based Distributed Hash-Table as Surrogate Model for HPC Applications", which appeared in the Proceedings of the 25th International Conference on Computational Science (ICCS) [12]. This extended version provides more details about the approaches, implementation, and evaluation of the MPI-DHT. Additionally, it includes a comparison of the MPI-DHT with the DAOS key-value store.

Surrogate models can play a pivotal role in enhancing performance in contemporary High-Performance Computing applications. Cache-based surrogates use already calculated simulation results to interpolate or extrapolate further simulation output values. But this approach only pays off if the access time to retrieve the needed values is much faster than the actual simulation. While the most existing key-value stores use a Client-Server architecture with dedicated storage nodes, this is not the most suitable architecture for HPC applications. Instead, we propose a distributed architecture where the parallel processes offer a part of their available memory to build a shared distributed hash table based on MPI. This paper presents three DHT approaches with the special requirements of HPC applications in mind. The presented lock-free design outperforms both DHT versions which use explicit synchronization by coarse-grained resp. fine-grained locking. The lock-free DHT shows very good scaling regarding read and write performance. The runtime of a coupled reactive transport simulation was improved between 14% and 42% using the lock-free DHT as a surrogate model.

Keywords: Distributed Hash Table · Key-Value Store · Surrogate Model · RDMA · DAOS

1 Introduction

During the last years, several research groups have shown the benefit of surrogate models for accelerating parallel simulations [2, 3, 9, 20]. While Raissi et al. [20] propose *physics-informed neural networks*, De Lucia et al. use *decision trees* to speed up geochemical simulations [3]. Reaktoro [9] and POET [2] make use of fast caches within their surrogate approach. Reaktoro uses so called *On-Demand Machine Learning* (ODML) to speed up chemical calculations. ODML works by extrapolating new chemical states of multiphase systems undergoing chemical reactions. Given new inputs, Reaktoro's ODML looks up a past calculation for which the Jacobian is known and estimates the output using Taylor extrapolation [9]. POET is a coupled reactive transport simulation which uses a distributed hash table (DHT) as fast storage for simulation results. These are reused to approximate further results in subsequent time steps. An *approximated lookup* is used where the modeler has to specify a possible rounding for each variable. Thus, there is a tradeoff between performance and modeling accuracy. Such cache-based surrogates work fine as long as the query and retrieval times are much faster than the full physics geochemical simulations.

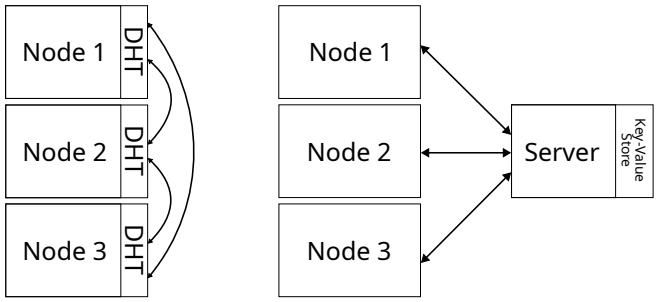
Starting with the relevance of key-value stores in the context of big social media applications, see for example Facebook [18], researchers spent great effort to improve the performance. One of the first steps was to accelerate the communication by introducing RDMA-capable networks [1, 2, 4, 5, 7, 8, 15, 17]. All these RDMA-capable approaches have in common that they have to solve three problems:

1. Design of **Addressing**: For an RDMA operation, the source has to know the physical address of the object where to read resp. write the data on the target side. Some systems use a special *index table* which stores the mapping between key and address [1, 22]. Others use a *direct hashing* where the physical address is directly derived from the key [2]. In case of a client-server architecture, the address information is exchanged via a Remote Procedure Call (RPC) in advance [6, 8, 11].
2. Design of **Data Consistency**: Since read and write operations may occur concurrently, there must be taken care of data consistency. This is done by a server (central approach) [4, 6, 8, 11], a synchronization protocol (for example Readers & Writers) [2], or using checksums for self-verifying data structures [17, 22].
3. Design of **Collision Handling**: There exist several collision handling strategies. For example, Hopscotch hashing implemented by FaRM [4] or Cuckoo hashing implemented by Pilaf [17] and LFBCH [10].

MPI is the de facto standard in HPC and also offers an API for Remote Memory Access (RMA). Hence, it is a straightforward idea to implement the key-value store using the MPI RMA API and to benefit easily from the experiences and improvements of the HPC community (see for example [2,5,15]). With every optimization in the MPI library, DHTs can profit from it without the necessity

of reimplementation in a self-made communication layer. In an earlier work, we integrated an MPI-based DHT, called MPI-DHT in the following, into the coupled reactive transport simulator POET as a surrogate model [2].

Most key-value stores are server-based, see for example [4, 7, 8, 11, 17]. However, this architecture is not the most suitable for HPC applications because it requires additional hardware and setup as shown in Figure 1. Further, Figure 1 shows the different communication patterns of a fully distributed and a server-based key-value store. While in the server-based approach, the clients always communicate with a central server, in the fully distributed approach clients may access the data directly from remote storage, e.g. using RDMA operations. The benefit of the central server approach is data consistency, while in the distributed approach data consistency can only be achieved by additional synchronization protocols. This paper discusses fully distributed key-value store architectures based on MPI that allow seamless integration into scientific applications.



(a) Fully Distributed (b) Server-based

Fig. 1. Comparison of distributed and server-based key-value stores.

The contributions of this work are:

- A performance comparison of the MPI-based DHT (MPI-DHT) from [2] and the server-based key-value store DAOS [11]. Despite a scaling problem, the distributed architecture of the MPI-DHT performs much better than the server-based DAOS architecture.
- Presenting two additional distributed hash-table architectures based on the MPI one-sided communication API, including a fine-grained locking DHT, and one lock-free approach which uses optimistic concurrency control.
- An evaluation of all three DHT approaches with a synthetic benchmark testing the DHT read and write performance shows the performance advantages of the lock-free approach by a factor of up to 1,400.
- The lock-free DHT scales very well, both for read and write requests. For 640 participating processes, 16 Million read operations per second and 15 Million write operations per second were observed.

– The DHT was integrated as fast data cache into a coupled geochemical transport simulation. In case of the lock-free DHT, the runtime was improved by 42% running on 128 cores, and by 14% running on 640 cores.

2 Related Work

Since more than one decade, researchers investigate implementation possibilities for key-value store and DHTs which exploit the capabilities of modern networks.

Gerstenberger et al. presented a distributed hash table using MPI RMA for the Cray Gemini and Aries interconnects [5]. For the coordination of reader and writer processes, they use MPI's passive target synchronization with a best effort approach: If a lock acquisition does not succeed, all data structures will be released and the process will try again later with an exponential back off. This is implemented within their own MPI-3.0 RMA library implementation optimized for the Cray Gemini and Aries interconnects where inserts are based on atomic compare and swap (CAS) and atomic `fetch_and_op` operations which are implemented on top of proprietary Cray-specific APIs. The measurements demonstrate the scaling of the implementation on up to 32k cores on the Cray machine. Another MPI-based distributed hash table is the MDHIM key-value store [6]. The evaluation shows that it outperforms the Cassandra key-value store which is common in the field of Big Data using a uniform distribution. MDHIM does not exploit the RDMA capability of the underlying network. Instead, each MPI process starts a so-called Range Server which serve client requests.

There exist several key-value stores leveraging RDMA. Pilaf [17], FaRM [4], and HERD [8] have a server-based architecture which is not suited for HPC environments. Instead, we investigate different DHT implementations which have a fully distributed architecture. The MPI-DHT versions which are discussed in this paper implement the read operation similar to the Cuckoo hashing approach from Pilaf, as we provide multiple indices where a value might be stored. However, our implementation does not require any movement of buckets during a write process, as seen in Cuckoo hashing [1, 17] or hopscotch hashing [4].

Nessie also uses RDMA read and write operations, but it has a distributed architecture. Further, Nessie is designed to efficiently support large data values up to several kilobytes [1]. Therefore, Nessie decouples indexing metadata, so-called index tables, and the key-value pairs. To ensure consistency, Nessie uses atomic swap operations on the index table.

In the following we present different MPI-based DHT implementations which all use RDMA for read and write accesses.

3 Comparison of MPI-DHT and the Key-Value Store DAOS

Available implementations for production use in HPC are rare. An exception are the MPI-DHT, and the DAOS implementation[4]. DAOS stands for Distributed

[4] `https://github.com/daos-stack/daos`

Asynchronous Object Storage and is an open-source server-based object store designed by Intel for distributed Non-Volatile Memory (NVM) technologies [11]. We conducted a comparative evaluation between the MPI-DHT [2] and the server-based approach DAOS.

Next we describe the key design features regarding addressing, data consistency and collision handling of the two systems.

3.1 Coarse-Grained Lock-Based MPI-DHT

The MPI-DHT API [2] consists of only four operations: `DHT_create, DHT_read, DHT_write` and `DHT_free`. The `DHT_read` and `DHT_write` operations are implemented using MPI's one-sided communication operations `MPI_Put` resp. `MPI_Get` to access the remote memory.

The original MPI-DHT implementation utilizes MPI's passive target synchronization, leveraging `MPI_Win_lock` and `MPI_Win_unlock` operations [2]. Each participating process allocates memory using `MPI_Window` to share it with the other application processes. The memory window is subsequently divided into multiple buckets. Each bucket contains a key-value pair and an additional Byte for meta information, such as an *occupied* flag. Thus, this approach requires only one additional Byte per bucket.

Addressing: The address of a bucket is a pair consisting of the process rank (target rank) holding the data and an index within the memory window. First, a 64-bit hash sum of the key is generated. A modulo operation by the total count of participating processes is used to determine the target rank.

Collision Handling: A set of bucket indices is derived from the hash sum by dividing the hash into smaller parts. Given an index of size n bytes and B buckets per memory window, we choose n as the smallest integer that satisfies the inequality $log_2(B) \leq 8n$.

Figure 2 shows an example where a 3-byte index is used which allows a memory region with a maximum of $2^{8 \cdot 3} = 2^{24}$ buckets. By moving forward by 1 Byte, 6 different bucket indices are derived at which a key-value store can be stored in the memory window of the target rank.

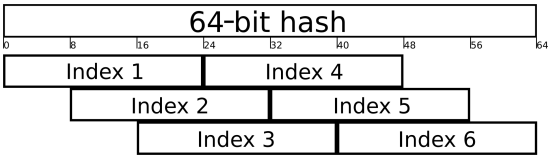


Fig. 2. Determination of addresses of a bucket in the MPI-DHT. [2].

In the context of a write operation, the target rank and the corresponding bucket indices are calculated, and then the first bucket is checked using `MPI_Get`. If the meta information is not set to *occupied*, data are written to the bucket

using `MPI_Put`. The data consist of the key-value pair and the meta information where the *occupied* flag is set. In the event that the bucket is already *occupied*, but the requested key matches the current key in the bucket, the value is updated. If the key does not match, the bucket at the next index is checked. This process is repeated until an empty bucket or a bucket with the same key is found. If the last index is reached and no empty bucket or updatable key was found, this bucket is overwritten.

The read operation employs a similar scheme, traversing all possible buckets of the target rank. It is checked, whether a bucket is *occupied* and whether the key matches the requested key. If a match exists, the value is returned.

Data Consistency: The MPI-DHT implements a Readers&Writers semantic. Whenever an `DHT_read` or `DHT_write` operation is initiated on a target rank, the entire memory window of the target rank is locked with `MPI_Win_lock`. Depending on whether the operation is a `DHT_read` or `DHT_write` operation, the window is locked in *shared* or *exclusive* mode. The lock is released with `MPI_Win_unlock` after the operation is completed. Since always the entire memory window is locked, we call it the coarse-grained MPI-DHT.

3.2 DAOS

The DAOS server is responsible for determining memory addresses, ensuring the consistency of data, and handling collisions. The protocol initiates with a request message to the server. In the case of a read operation, the server is informed of the location on the client side where the data is to be written and initiates an RDMA `PUT` operation. In the case of a write operation, the message includes the address on the client side where the data is to be retrieved. The server then retrieves the key-value pair to be stored by a subsequent call to a RDMA `GET` operation. After all RMA operations have been completed, the server sends a reply message to inform the client that the requested operation is finished.

The DAOS protocol differentiates between small and large messages. For messages smaller than 18 kilobytes, the initial request message already contains the data to be written or read, thus eliminating the need for additional RMA operations on the server side.

3.3 Test bed and Benchmark Description

We conducted the evaluation on four nodes of the Turing Cluster at the University of Potsdam. Each node is equipped with two Intel Xeon E5-26540v4 processors with 12 hardware cores each, 64 GBytes of main memory, and interconnected through RoCE ConnectX-6 Dx 100 Gbit NICs.

The nodes were configured with Rocky Linux 8.8 and Mellanox OFED driver version 1.0.1. One node hosted the DAOS server, while the remaining three nodes served as clients. Since the MPI-DHT stores the values into the RAM, DAOS was also configured to use non-persistent RAM as key-value storage. For the MPI-DHT measurements, Open MPI version 4.1.5a1 was used.

We measure the operations per second (OPS) for `Read` and `Write` operations separately across varying numbers of clients. For the DAOS evaluation, we utilized the KV-API of the library to interact with the server. The key and value sizes were set to 80 bytes and 104 bytes, respectively, in accordance with the requirements of the chemical simulation described in the POET evaluation [2], which is greater than the 16 byte key and 32 byte value sizes used for the evaluation of other key-value stores [4, 8, 22]. Keys were randomly generated using a uniform distribution where every client starts with a different seed. Each client executes 100,000 write operations and then reads all 100,000 written entries. The median read and write performance of five repetitions are presented without error bars, as the maximum coefficient of variation is 3.8%.

The benchmark was scaled from 12 to 72 clients, with an increase of 12 clients per step. The processes were mapped onto a node in a dense manner, resulting in the filling of one NUMA node after another. For the distributed MPI-DHT, each client contributed 1 GByte of its memory to the DHT.

3.4 Results: Read/Write Performance

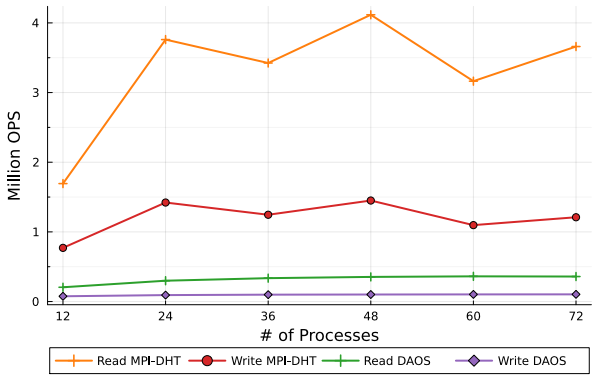


Fig. 3. Throughput of DAOS and MPI-DHT for *read* and *write* operations

Obviously, the MPI-DHT outperforms DAOS in both read and write operations, as illustrated in Figure 3. The MPI-DHT reaches its peak performance with 4.12 million reads and 1.45 million writes per second when utilizing two nodes (48 processes). The throughput of DAOS remains relatively constant and reaches its maximum read rate at 60 clients with 362 thousand operations per second and its maximum write rate with 103 thousand operations per second at 72 processes.

The median latency of the MPI-DHT is between 4 μs and 17 μs for read access and between 13 μs and 57 μs for write access. The latency of DAOS is between

56 μs and 198 μs for read and between 157 μs and 698 μs for write access. The factor of improvement of the MPI-DHT compared to DAOS lies between 8.2 - 12.5 for read and 10.1 - 15.3 for write operations.

Instead of scaling with the number of clients, MPI-DHT and DAOS demonstrate both a stagnation in throughput. The poorer DAOS performance can be attributed to the central approach and indicates the server as the bottleneck of the setup. The performance of the MPI-DHT is deeper analyzed in the following.

3.5 Discussion of MPI-DHT Performance

We identified the synchronization overhead caused by the explicit locking of a target window as specified by the MPI standard as the bottleneck. To be concise, for 72 processes 80 % (`DHT_write`) resp. 48 % (`DHT_read`) of one call are spent in `MPI_Win_Lock` and `MPI_Win_Unlock`. There are two reasons for this high synchronization overhead. Firstly, the MPI-DHT treats the entire DHT memory of one process as a single window, which results in the unnecessary locking of the entire memory while only one bucket is accessed. Secondly, in the Open MPI implementation, the locking mechanism involves busy-waiting loops utilizing compare-and-swap, atomic fetch, and atomic fetch-and-add operations to facilitate exclusive and shared locking. However, this busy-waiting loop can potentially generate substantial network traffic in typical Readers & Writers scenarios where the target memory is either exclusively locked or intended to be exclusively locked, but shared locks are already acquired.

Given these limitations, we propose two new DHT synchronization approaches.

4 Improving Synchronization Methods for Distributed Hash Tables with MPI

The following presents two new approaches to address the data consistency problem of the MPI-DHT:

- A *fine-grained locking* MPI-DHT which uses MPI's atomic operations.
- A *lock-free* MPI-DHT with optimistic concurrency control. It uses `MPI_Put` and `MPI_Get` operations without any synchronization/locking. Instead, checksums are used to detect conflicts. This approach is adapted from Pilaf [17].

The decision to continue using the MPI library for the implementation of the DHT was guided by its status as the de facto standard in HPC environments. This ensures the library's availability to a broad user base and provides a "plug-and-play" solution for every MPI-parallelized application.

The two new MPI-DHT variants are discussed in detail in the following sections.

4.1 Fine-Grained Locking MPI-DHT

Regarding *addressing* and *collision* handling, the coarse-grained locking (see Section 3.1) and the fine-grained locking MPI-DHT are identical.

Data Consistency: Instead of locking the entire memory window of the target rank, the fine-grained locking mechanism locks only the bucket that is currently to be accessed. One way to approach this is to define a memory window for each bucket. This naive implementation would lead to a massive overhead in terms of memory consumption, as each memory window would return a data struct with a size dependent on the MPI implementation. For Open MPI version 5.0.2, this would result in a memory overhead of 352 bytes per bucket. This is not feasible for numerous buckets. Therefore, the implementation uses self-implemented locking on 8 byte integers and relies on `MPI_Compare_and_swap` and `MPI_Fetch_and_op` operations. The implementation is adopted from the Open MPI implementation of passive-target synchronization which uses UCX atomic operations.[5] In order not to violate the MPI standard by performing RMA operations outside an epoch [16, p. 588], all windows are *shared* locked beforehand by all processes with `MPI_Win_lock_all`. This was inspired by the approach employed by Schuchart et al. in their work on a lock-free message queue [21].

A lock value of $0x10000000$ means that a writer is active on this bucket (*exclusive lock value*). To acquire this exclusive lock, a write process attempts to set the lock atomically to $0x10000000$ if the current value is set to zero by employing the `MPI_Compare_and_swap` function. This is repeated until the lock is acquired.

Readers only have to register their read interest. Therefore, a reader process attempts to increment the lock atomically by one using the `MPI_Fetch_and_op` function until the lock is acquired. The acquisition of the lock is defined as successful, when the value prior to the increment is less than $0x10000000$ (exclusive lock value). However, if the value is greater than or equal to the exclusive lock value, the origin process must revoke its read request by decreasing the lock value again and attempting to acquire the lock once more. This guarantees that multiple readers can access the same bucket concurrently, while only one writer can access the bucket at a time.

The release of a lock is initiated by the origin process, which performs a decrement on the lock value by the exclusive lock value (writer) or by one (reader), respectively.

In order to facilitate the locking mechanism at the bucket level, an 8-byte lock is incorporated into each bucket, which is initialized to 0. Due to the requirement that locks be aligned to a multiple of 8 bytes, a padding of up to 7 bytes may be necessary. This results in a maximum overhead of 15 bytes per bucket in comparison to the coarse-grained locking MPI-DHT.

[5] `https://github.com/open-mpi/ompi/blob/v5.0.6/ompi/mca/osc/ucx/osc_ucx_passive_target.c`

4.2 Lock-Free MPI-DHT

As with the fine-grained locking mechanism, the lock-free MPI-DHT implementation utilizes the same addressing and collision handling method as previously defined. However, the locking mechanism is substituted by a checksum calculation inspired by the work of Pilaf [17]. Rather than adding bytes for a lock, each bucket contains an additional 32-bit value for storing a checksum.

Data Consistency: In case of a `DHT_write` operation, the origin process is responsible for calculating a checksum of the key-value pair and appending it to the bucket data.

Subsequently, a reading process retrieves the bucket data and recalculates the checksum. If the recalculated checksum is equal to the stored checksum in the bucket, the key-value pair is returned to the application. In the event of a mismatch, the `MPI_Get` operation and checksum check is repeated. If the checksums persist in diverging, the bucket is flagged as *invalid* in the meta information field. In the event that a write operation is initiated on an invalid bucket, the bucket can be overwritten with the new key-value pair.

This checksum-based approach is a lock-free mechanism that ensures the data consistency of the MPI-DHT. Consequently, it does not require additional atomic operations or locks. As discussed in Section 4.1, all windows are locked by all processes with `MPI_Win_lock_all` prior to any RMA operation.

5 Evaluation of the MPI-DHT with Different Synchronization Methods

The next section describes our test bed. Then we present results with synthetic benchmarks to investigate the different behavior for read and write requests. This is done for two different benchmarks (uniform and zipfian distribution) to test the influence of the distribution of bucket accesses. Finally, we present results where all three MPI-DHT variants were tested as surrogate model within the reactive transport simulator POET [2].

5.1 Test Bed

All the benchmarks were conducted on the cluster of the Potsdam Institute for Climate Impact Research (PIK)[6], Germany. Each node is equipped with two AMD EPYC 9554 CPUs, each possessing 64 cores and a base clock speed of 3.1 GHz. In all experiments, a dense mapping is used where all 128 cores of a node are used.

Both CPUs share a total memory capacity of 768 GB, with dual-ranked DDR5 memory being utilized. The nodes are interconnected via NVIDIA Mellanox ConnectX-7 NDR Infiniband, which provides a data transfer rate of 400 Gbps per port.

[6] `https://www.pik-potsdam.de/en/institute/about/it-services/hpc`

For the execution of all experiments, the GNU Compiler Collection in version 14.1 was employed. The Message Passing Interface (MPI) library of choice was Open MPI version 5.0.6, accompanied by an UCX version of 1.17.0. The code was compiled with the flags `-O3 -DNDEBUG`.

Furthermore, to enable Open MPI to utilize a single atomic remote memory operation across the Infiniband network, the parameters `osc_ucx_acc_single_intrinsic` and `osc_rdma_acc_single_intrinsic` were set to true.

5.2 Synthetic Benchmarks

First experiment: The objective of the first benchmark is to evaluate the maximum throughput of only read and write operations, respectively. To this end, a benchmark was designed to generate a random number from which an 80-byte key is derived. The value size is set to 104 bytes. The sizes were selected to model the size of a typical key-value pair in the geochemical simulation POET [2]. For random number generation, both uniform and zipfian distributions were employed. The zipfian distribution with a skew of .99 and a range from 1 to 712,500 was chosen, since it models best the distribution of access requests within the POET simulation.

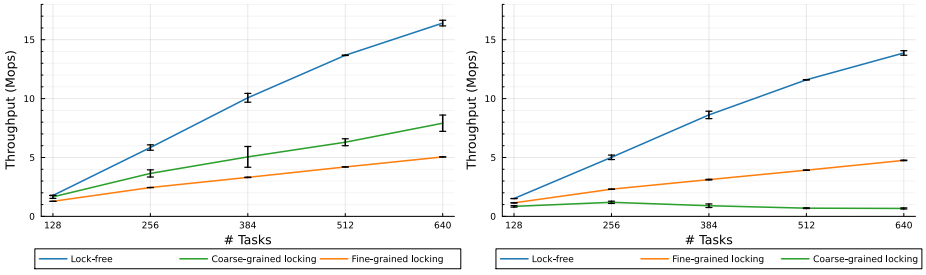
The benchmark generates 500,000 key-value pairs and writes them into the DHT. After the completion of the write phase by all benchmark processes, the same-key value pairs previously written are read by each process. For both blocks, the throughput is calculated as the number of operations per second.

Second experiment: The second benchmark is designed to evaluate the performance of a mixed benchmark that is more read-intensive. For this, a process performs 1,000,000 operations consisting of 95% reads and 5% writes. The ratio also derives from the access pattern of the geochemical simulation [2]. The throughput is calculated as the number of operations per second, combining both reads and writes.

5.3 Results with Synthetic Benchmarks

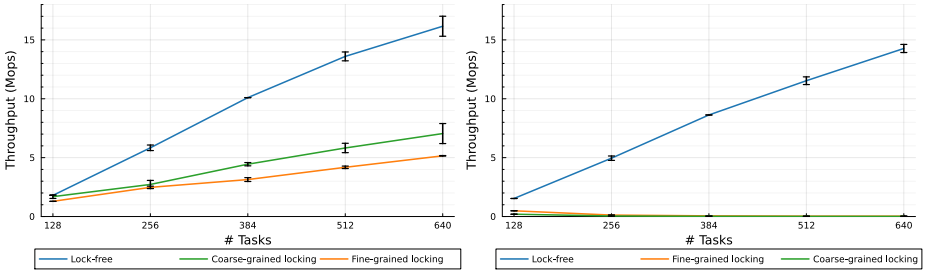
We varied from 1 to 5 nodes with densely mapped NUMA nodes, leading to a maximum of 640 processes. Each process provides 1 GB of memory for the DHT. The benchmark was replicated five times, and the median values of the throughput for read-only and write-only operations, respectively, along with their respective standard deviations, are displayed in Figures 4a and 4b for the uniform distribution, and in Figures 5a and 5b for the zipfian distribution.

For the read-only and write-only benchmarks, both uniform and zipfian distributions, the throughput of the lock-free DHT is significantly higher than both synchronized approaches. For example, in case of 640 processes the lock-free MPI-DHT performs 16.4 (uniform distribution) resp. 16.2 (zipfian distribution) million `MPI_READ` operations per second. This is about 3 times higher than fine-grained locking and 2 times higher than coarse-grained locking. Comparing read and write requests, the throughput of write operations is always lower than that of read operations for all approaches. This is expected since a write operation



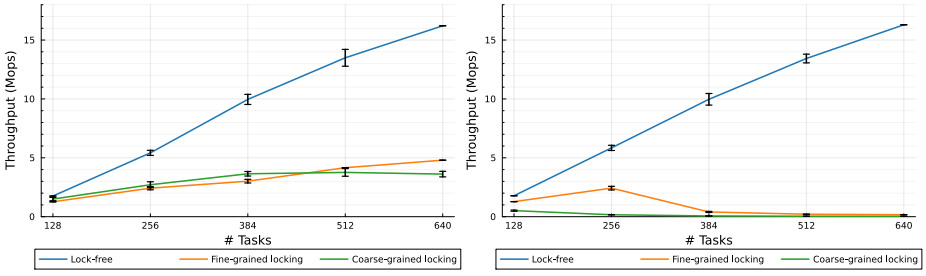
(a) Read only (b) Write only

Fig. 4. Throughput of read and write operations with *uniform* distributed keys.



(a) Read only (b) Write only

Fig. 5. Throughput of read and write operations with *zipfian* distributed keys.



(a) Uniform Distribution (b) Zipfian Distribution

Fig. 6. Throughput of mixed benchmark with a 95% Read/5% Write ratio for uniform and zipfian distributed keys.

requires at least one additional read operation to determine whether the bucket is writable or matches the requested key to update the value.

Table 1. Write-only Performance for 640 Processes in Million Operations per Second.

Benchmark	**Coarse-Grained**	**Fine-Grained**	**Lock-Free**
uniform	0.67	4.75	13.9
zipfian	0.01	0.03	14.3

Table 1 shows the write-only performance for 640 processes. This demonstrates clearly the high overhead of the locking mechanisms. For uniformly distributed keys, the lock-free MPI-DHT performs about a factor of 2.9 times better than fine-grained locking, and about 20.6 times better than coarse-grained locking. For the zipfian distribution, the lock-free MPI-DHT is even 477 times better than fine-grained and 1430 times better than coarse-grained locking. Here, the fine-grained locking mechanism shows it advantage of not blocking other write operations destined for other buckets within the same memory window.

For the mixed load benchmark, the throughput of the lock-free DHT is in case of 640 processes 16.2 (uniform distribution) resp. 16.4 (zipfian distribution) which is near its read-only performance. For the uniform distribution, the performance of the fine-grained locking increases to 4.7 Mops compared to 3.6 Mops for coarse-grained locking. Evidently, a zipfian distributed key challenges both synchronized approaches. While fine-grained locking only increases from 1.27 to 2.42 million operations per second for 128 to 256 processes, coarse-grained locking even degrades from 0.51 Mops to 0.17 Mops for the zipfian distribution.

The number of reads that failed due to an invalid bucket caused by a checksum mismatch as described in Section 4.2 is shown in Table 2. It can be seen that the read-only benchmark does not produce any checksum mismatches, nor does the mixed load benchmark with uniformly distributed keys. In fact, only zipfian's distributed key generation results in reading corrupted data, caused by two or more processes writing to a bucket at the same time. It also shows that the absolute number of checksum mismatches increases as the number of processes increases. However, these mismatches can be neglected because the number is very small in relative terms.

Table 2. Checksum mismatches for the lock-free DHT.

Benchmark	**# of Tasks**	**# of Mismatches**	**Percentage [%]**
mixed - zipfian	128	13	$1.1 \cdot 10^{-5}$
mixed - zipfian	256	16	$6.5 \cdot 10^{-6}$
mixed - zipfian	384	25	$6.8 \cdot 10^{-6}$
mixed - zipfian	512	31	$6.3 \cdot 10^{-6}$
mixed - zipfian	640	64	$1.1 \cdot 10^{-5}$
Others	Any	0	0

5.4 HPC Use-Case: POET

POET [2] is a coupled reactive transport simulator parallelized by MPI that combines the flow and transport of solutes in porous media with geochemical reactions. The version used implemented an explicit upwind advection scheme as transport with constant fluxes on a 500×1500 grid, homogeneous in species concentrations. The same chemistry setup as described in [2] was used. The simulation was started with a constant injection of magnesium chloride by advection from the top left boundary of the grid. As the magnesium concentration increases, the previously equilibrated calcite begins to dissolve and dolomite precipitates. Once calcite is completely consumed, dolomite also starts to redissolve. POET reuses PHREEQC [19] to simulate these kinetic processes.

Due to the advective transport, a sharp reaction front can be observed during the runtime of the simulation, while cells not yet reached by the reactive solution remain unchanged. This makes it possible to cache previously simulated results, e.g. in a distributed hash table. POET already implements caching with the proposed DHT-API.

To cache simulation results, the input parameters for the geochemical simulation are rounded to a user-defined number of significant digits to serve as key for the DHT. These are 9 species and the simulation time step, represented as double values. The stored value data consist of the exact result simulated by PHREEQC together with the given input, accounting for another 13 double values. Thus, the key-value pair has a size of 80 bytes for the key and 104 bytes for the value.

The simulation was started with 500 time steps, where for each time step first the flux (in this case constant fluxes), the transport (upwind advection) and the geochemical reaction (PHREEQC) were simulated. There is actually one chemical simulation per grid cell per time step. Whenever a cell is simulated by PHREEQC, the result is stored in the DHT, and a next call with approximately the same input to the time-consuming simulator can be avoided by retrieving the value from the DHT.

Again, the simulation was scaled from 1 to 5 nodes, densely populated with one MPI task per CPU core. Each experiment was repeated three times for the three DHT approaches, and a reference without any DHT enabled. The median runtimes of the chemical simulation, along with the respective standard deviation, are shown in Figure 7. For this particular simulation setup, the average hit rate over all DHT runs was 91.8%.

The coarse-grained locking DHT was a very good improvement in the experiments presented in [2]. The picture is now completely different on the newer hardware (see Section 5.1) and with the newer faster POET version. Now, only the lock-free DHT actually has a positive impact on the runtime of the simulation.

The coarse-grained locking MPI-DHT slows down the application and shows the worse runtime compared to the reference run for all node counts. This approach also shows the highest variation between repeated simulation runs.

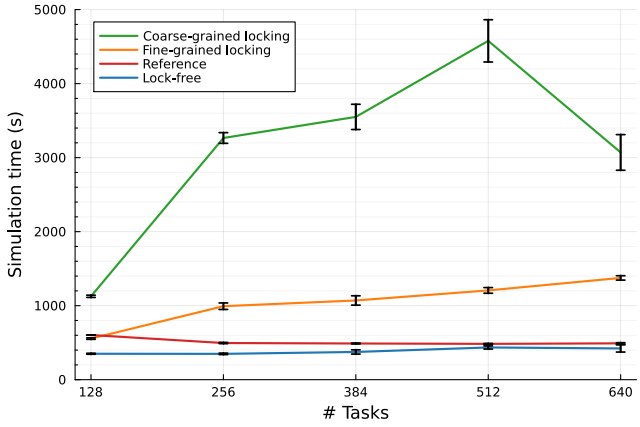


Fig. 7. Runtime of the chemical simulation of POET w/ and w/o DHT.

Table 3. Performance gain of the POET simulation with lock-free MPI-DHT compared to the Reference Run without DHT.

# of Tasks	Performance Gain
128	41.9%
256	29.5%
384	23.3%
512	10.1%
640	14.1%

The fine-grained locking MPI-DHT shows only a slight improvement for 128 processes, while increasing the number of nodes also degrades the performance compared to the reference run.

Furthermore, since increasing the number of processes has only a small impact on the runtime of the reference run from 603 seconds for 128 processes to 491 seconds for 640 processes (speedup of 1.23 compared to the runtime on 128 cores), it can be assumed that the simulation has already reached the maximum degree of parallelization when using only one node. Nevertheless, the lock-free DHT is still able to reduce the runtime of the simulation. The best result is achieved for 128 processes reducing the simulation time from 603 seconds to 350 seconds compared to the reference run. Table 3 shows the performance gain for the different numbers of tasks.

Further, we investigated the number of mismatches which occurred during the simulations with the lock-free DHT (see Table 4). The maximum checksum mismatches are 4421 for 640 processes, which means that only 0.0013% of all read requests were corrupted.

Table 4. Checksum mismatches for POET simulation (lock-free MPI-DHT).

# of Tasks	# of Mismatches	Percentage [%]
128	1507	$4.4 \cdot 10^{-4}$
256	3049	$8.9 \cdot 10^{-4}$
384	4315	$1.3 \cdot 10^{-3}$
512	2884	$8.4 \cdot 10^{-4}$
640	4421	$1.3 \cdot 10^{-3}$

6 Conclusion and Future Work

While server-based distributed key-value stores are more common, the setup and maintenance costs of dedicated hardware are questionable. In a preliminary study, Intel's server-based solution DAOS was outperformed by the distributed solution MPI-DHT with coarse-grained locking. However, the MPI-DHT had scaling issues due to synchronization overhead.

Due to this fact, this paper investigates three MPI-Based DHT implementations with different approaches to achieve data consistency: a coarse-grained locking DHT, a fine-grained locking DHT, and a lock-free DHT with checksum validation.

First, an evaluation of these approaches was performed using a synthetic benchmark. The lock-free DHT outperformed both locking DHT approaches in terms of read and write performance, with throughput improvements of up to 3 times for read operations and up to 1,400 times for write operations.

The evaluation was extended to a real-world application where all three approaches were integrated into the reactive transport simulator POET as a surrogate model. Only the simulation runs with the lock-free DHT showed runtime improvements compared to the simulation without DHT. The runtime of POET was reduced by 14% up to 42% depending on the number of processes.

The MPI-DHT does not support runtime table resizing. However, resizing could be managed during HPC application check pointing, adjusting the table size on restart. In the experiments, only the Open MPI implementation was used. A deeper analysis of the performance of different MPI implementations will be considered in future work. Further, experiments with different sizes of data values will be of interest.

In the experiments, the lock-free DHT impressed with a performace of 16 Million read operations per second and 15 Million write operations per second. This makes the lock-free DHT suitable as a fast data cache within HPC applications.

The benchmark code and data are published on Zenodo [13] and the MPI-DHT implementations are available as open-source software [14].

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