Hardware locality-aware partitioning and dynamic load-balancing of unstructured meshes for large-scale scientific applications

Pavanakumar Mohanamuraly
mpkumar@cerfacs.fr
CERFACS
Toulouse, France

Gabriel Staffelbach
gabriel.staffelbach@cerfacs.fr
CERFACS
Toulouse, France

ABSTRACT
We present an open-source topology-aware hierarchical unstructured mesh partitioning and load-balancing tool TreePart. The framework provides powerful abstractions to automatically detect and build hierarchical MPI topology resembling the hardware at runtime. Using this information it intelligently chooses between shared and distributed parallel algorithms for partitioning and load-balancing. It provides a range of partitioning methods by interfacing with existing shared and distributed memory parallel partitioning libraries. It provides powerful and scalable abstractions like one-sided distributed dictionaries and MPI3 shared memory based halo communicators for optimising HPC codes. The tool was successfully integrated into our in-house code and we present results from a large-eddy simulation of a combustion problem.

CCS CONCEPTS
• Computing methodologies → Massively parallel and high-performance simulations; Massively parallel algorithms.

KEYWORDS
Hardware-aware load-balancing, MPI3 shared memory, topology-aware hierarchical algorithms, unstructured mesh partitioning

ACM Reference Format:
Pavanakumar Mohanamuraly and Gabriel Staffelbach. 2018. Hardware locality-aware partitioning and dynamic load-balancing of unstructured meshes for large-scale scientific applications. In PACS ’20: Platform for Advanced Scientific Computing, June 29–July 01, 2020, Geneva, Switzerland. ACM, New York, NY, USA, 10 pages. https://doi.org/10.1145/1122445.1122456

1 INTRODUCTION
The road to exascale has many facets, on the one end are the challenges of hardware resilience and data storage and on the other is the challenge of scaling existing scientific software on exascale hardware. Heterogeneous architectures (accelerators) with hybrid parallelisation techniques so far have shown good promise but come with many drawbacks. The first problem is the shear abundance of hybrid programming models. Every HPC vendor seem to have a solution: Intel OneAPI [37], Kokkos [9], RAJA [21], Intel TBB, Charm++ [41], CUDA, Chapel [11], etc. Even standards are many OpenMP, OpenACC, OpenCL, OMPI, etc. Most times features from a latest version or standard is necessary for better performance but might not be portable. Also some of theses models have a steep learning curve to write performant code. This leads us to the second major problem of portability (of both platform and performance). The third major problem is the issue of software maintenance since the programming models require major disruption to the code to achieve best performance.

Even though one has a variety of choices for the SMP computing the choice is quite limited for the off-processor model. In fact MPI is the de facto standard. The success of MPI has been its simplicity and portability. Armed with just few MPI calls it is possible to run the code on both SMP and off-processor nodes. But the MPI implementations have remained stagnant and have responded only when challenged by competing programming models. In addition safely mixing SMP models with MPI is still problematic with little or no debugging support for an application developer. For example supporting MPI calls inside threads/tasks is still unsupported in many vendor MPI libraries and not widely portable or available.

Nevertheless, with the advent of the wide adoption of the MPI3 and maturity of the library ecosystem it is now possible to mitigate most of the performance problems associated with a pure MPI implementation. The Exascale MPI and OMPI-X projects have already begun to address the various needs of exascale computing and the MPI4 standard is in the making. Rafenetti [32] shows the various optimisations undertaken in MPICH2 library to mitigate issues with large number of MPI process or ranks. Balaji [3, 39] et al. discuss running MPI on millions of cores and provide techniques to alleviate scalability limitations in applications.

Our in-house HPC combustion code AVBP[17, 18, 35] is a conglomerate effort of several years of research and development. It has many stakeholders ranging from universities, research labs and industrial partners. Therefore we exercise extreme prudence before bringing disruptive changes since every change must be validated across our value chain. We investigated the sources of the issues associated with running MPI on many ranks (typically 10k-15k). We found satisfactory solutions without resorting to hybrid-programming and with minimal disruption to our code. To our surprise every solution revolved around one theme, locality-awareness.

We organise the paper as follows: (i) outline the problems associated with MPI for large number of ranks, (ii) present TreePart library and standalone tools which are aimed at solving most of the...
aforesaid problems, and (iii) substantiate with results from our in-house code AVBP (iv) followed by an outline on our future direction of research.

2 PROBLEMS WITH MPI SCALING
Parallel unstructured mesh solvers behave much differently when compared to structure or multi-block structured meshes. The computation in the case of unstructured meshes are irregular causing problems of indirect, non-strided, or non-contiguous access to memory. In addition they require the use of more sophisticated tools to partition the mesh. Structured mesh problems are much easier to tune and hence tuned library implementations are ubiquitous. This is hardly true in the case of unstructured meshes. A summary of the most critical performance problems running parallel unstructured mesh based solvers is shown with relevant results.

2.1 Graph partitioning at scale
When the problem size (mesh size) becomes quite large the memory requirements of serial graph partitioning no longer fit even on a fat-memory node. Therefore, distributed graph libraries like ParMETIS [24], PT-Scotch [12], KaHIP [36], Zoltan [6], etc., are employed for partitioning the mesh. Mohanamuraly et al. [29] and Wang [40] et al. show that the quality of partitions (number of edge cuts) obtained from graph partitioning tools deteriorates rapidly when the number of partitions increases. In fact the partition quality considering the same underlying mesh using a parallel partitioner is worse than the serial algorithm [22].

In an online partitioning approach for unstructured meshes we ideally like to have every subscribed rank to participate and construct its local mesh. In our experience when we used core counts in excess of $5k$ (also MPI ranks) most graph partitioners fail due to the presence of all-to-all type communication in their implementation. Therefore we resort to an off-line partitioning strategy which limits the scope for online load-balancing and associated mesh partitioning. KaHIP [1] provides semi-external and external graph algorithms which can be used to partition very large meshes on a single rank but limits the scalability. In hybrid programming models the above problem is less severe (but still present) because the mesh is partitioned for physical nodes leading to lower partition counts.

2.2 Partition-to-rank assignment
This is an often overlooked problem in practical MPI implementations. Once a quality partitioning is obtained they have to be optimally placed or pinned to the physical cores reserved for the computation. Mapping each partition to MPI ranks in the natural ordering mostly results in poor performance. In figure 1 we show an unstructured mesh whose partitions are sub-optimally pinned to four nodes (with four cores each). Note that the core partitions (coloured red, pink, yellow, and green) in node 1 are scattered and share boundaries with many node neighbours. We also show an optimal node-to-rank placement in figure 2. MPI standard actually allows such optimised placement using MPI distributed graph topology [20, 33]. Unfortunately from our experience we never encountered an MPI library that actually does the optimal placement for distributed graphs. Similar observations were made by Hoefler et al. [19] who states that MPI mapping function are often not well implemented. Graph partitioning library KaHIP [36] provides optimal processor mapping of partitions by solving a sparse quadratic assignment problem. Note that hybrid programming models avoid this issue completely since the partitions are always at the node level.

2.3 Load imbalance
Load imbalance has been an important argument in favour of leaning towards hybrid programming compared to a pure MPI implementation. The runtime libraries like OpenMP, OpenACC, TBB, etc. automatically load-balance tasks/threads. But one needs to specify the right grain size for each task and the load-balancing strategy to obtain optimal performance. Usually the graph partitioner generates mesh partitions with an imbalance in element count within $1-2\%$. Certain additional operations like boundary conditions, numerical kernels that selectively execute based on solution evolution, contribute to additional load-imbalance. In figure 3 we show the load imbalance in our in-house code for an unstructured mesh with 150M tetrahedral elements, partitioned using ParMETIS, for different partition sizes. We clearly see a large imbalance in load even though the graph partitioner has under 2% vertex imbalance. Perfect load balancing is seldom possible in most CFD applications, especially when considering industrial configurations. A pure MPI implementation can suffer performance degradation since automatic load-balancing is not available in most MPI run time implementations except for AMPI, where the runtime calls user implemented packing/unpacking routines for automatic
migration of MPI process. Note that even in a hybrid environment node level imbalances cannot be mitigated as a result of this issue.

The load-balancing of tasks or threads in a hybrid model is highly essential and built into the run-time implementation. In the case of a pure MPI implementation a load imbalance would trigger a re-partitioning of the mesh or one needs to resort to the idea of over-subscription adopted by AMPI [41]. The over-subscribed case suffers even more with partition quality because the number of partitions are substantially higher than the partition-per-core MPI model.

Re-partitioning unstructured meshes to improve load imbalance requires the use of weights defined at mesh entities like nodes or elements. The weights are estimated using coarse grained measurements like compute time which need not directly correlate to the fine grain behaviour. In the presence of multiple computational kernels each exhibiting different or conflicting load imbalance it is impossible to accurately capture the behaviour using a single weight. A multi-constraint partitioning [23] is necessary to effectively handle such situations.

2.4 Intranode messaging

The intranode messaging is one of the most important performance optimisation in a pure MPI implementation. The three main approaches to MPI intranode communication are network loopback, user-level shared memory, and kernel assisted direct copy [10]. Network loop back has poor performance and seldom used nowadays. User-level shared memory is more widely implemented in MPI libraries. Kernel assisted direct copy approaches provide superior performance by eliminating intermediate copies. Linux kernel (v3.4 and above) has native support for Cross Memory Attach (CMA) to enable a single rather than a double copy of MPI messages via shared memory. CMA for intranode communication is supported by MPI libraries like Intel MPI, OpenMPI, etc. This is a less severe bottleneck on newer MPI implementations when direct kernel copy is supported by the kernel.

2.5 Communication imbalance

A major component contributing to imbalance in execution times between MPI ranks is communication imbalance. In figure 4 the IMB-MPI1 benchmark timing obtained for all-reduce and exchange is shown for inter and intranode placements. We see an almost tripling of network bandwidth in the case of intranode placement. Therefore even with an optimal placement of ranks to physical cores a pure MPI implementation suffers from performance degradation because the partitioner is unaware of this bandwidth difference and weights all communication equally as shown in fig. 5. Hence heavily optimised intranode communication actually amplifies the problem due to the large skewness in communication times. Contributing further to this imbalance is the difference between the send/receive message sizes across partitions. Overlapping communication with computation using non-blocking send/receive can mitigate communication imbalance. Situations do exist where overlap of communication and computation is impossible due to inherent synchronisations in the numerical implementation or this programming style needs extreme programming effort [30].

2.6 Redundant computations at halo entities

Most scientific codes based on MPI rely on halo entities to represent off-processor data necessary for local computations. Pre-conditioners based on the domain decomposition (for example
additive Schwarz) also employ large overlap in the partitions for convergence acceleration. However using overlapping (halo) entities introduces redundant computations resulting in an increase of the original problem size. Therefore the scalability of the code deteriorates because one now solves a larger problem compared to the original. In figure 6 the percentage increase in problem size ($\delta p$) for a 3D and 2D mesh with one layer and two layers of overlap is shown. With larger overlap we find that the partition size increases quite rapidly (larger slope) with processor count.

Hybrid programming has the advantage of employing lower number of partition counts. Hence for the same number of physical cores we considerably reduce redundant computations. Our in-house solver implements a cell-vertex finite volume scheme based on a zero-halo partitioning of the mesh i.e., zero overlapping elements. The numerical algorithm therefore contains almost no redundant computation making our solver extremely scalable and efficient. A zero-halo partitioning does produce redundant nodes or shared nodes across the partition boundary. But they only add to the memory overhead and not the computation time. We show a zero-halo partitioned mesh in figure 7 along with the shared nodes for reference.

2.7 Memory locality

Unstructured mesh solvers are mostly bandwidth limited and therefore sensitivity to memory locality. With an increase in partition count the data locality of irregular applications improve substantially resulting in excellent cache usage. Sometimes they even exhibit super-linear scaling because the problem fits perfectly within the cache block [34]. Usually data and computation reordering [27] is performed to mitigate such effects. Among such approaches the cache block partitioning (i.e., dividing the partition into cache block sizes) is found to be the most effective [14]. Hybrid implementations require colouring to avoid data dependencies in computational loops. Here each cache block size partition belonging to the same colour is concurrently run on independent threads of execution. In figure 8 we shown an unstructured mesh divided into cache blocks; (i) on the left are blocks distributed to 4 MPI ranks and (ii) on the right every block is partial distance-2 [15] coloured to remove data dependencies.

Clearly colouring destroys memory locality due to indirect addressing of data inside the loop. Lock and mutex are quite inefficient approaches to remove race condition and always avoided in computational loops. Pure MPI codes do not suffer from this problem because the mesh and associated data is contained in a given partition making memory access efficient. Virtually no difference in performance exists between threads and processes in a modern Linux operating system [4]. Therefore access to local variables, memory, instructions, etc., within a thread or within a process incur similar costs.

3 SOLUTIONS TO MPI PROBLEMS AT SCALE

Overall it is surprising to note that switching to a hybrid MPI approach does not solve any of the issues outlined in the previous
section except for the absence of internode messages. Problems are merely alleviated by reducing the number of MPI ranks. The issue of non-optimal processor placement is mostly due to the lack of an efficient distributed graph topology implementation in most MPI runtime. Therefore the choice of MPI vs. hybrid (MPI+X) is purely based on load imbalance and number of redundant computation. We feel that when an MPI code does not address the issue of load imbalance one cannot make a fair comparison between an MPI and hybrid (MPI+X) implementation. In fact fixing this issue will equally benefit MPI and hybrid (MPI+X) implementations.

Using static mesh partitioners as load balancers for unstructured meshes is a major bottleneck for MPI codes. Therefore we found a need for a dynamic load balancer with built-in hardware topology awareness. Hierarchical partitioning and load-balancing approach [25, 38] is quite effective in solving the major problems of (i) optimal partition placement, (ii) load/communication imbalance and (iii) online partitioning at scale. This motivated the development of the open-source topology aware hierarchical unstructured mesh partitioning tool TreePart to address these issues. We found only one open-source alternative namely Zoltan [13] for such purposes. Zoltan is now abandoned in favour of Zoltan2; which is still in development and lacks hierarchical partitioning support. In addition Zoltan is not hardware aware and contains MPI2 functions which are not scalable for many MPI ranks. For example the migration routines in Zoltan uses the inefficient MPI_AlltoAll and MPI_AlltoAllv functions. Also pack-unpack functions are used in many parts of the code which can mostly be avoided using MPI3 one-sided communication. In the next section we provide a brief introduction to the TreePart library and the algorithms implemented to enable scalable hierarchical mesh partitioning.

4 TREEPART OVERVIEW

TreePart is a topology-aware hierarchical unstructured mesh partitioning and load-balancing tool. It interfaces to existing partitioning tools like Zoltan, Metis, ParMetis, and PT-Scotch (support for KaHIP [36] is under development) and provides a scalable infrastructure for use in high MPI rank counts. Presently we tested the system up to 26k MPI ranks. The tool uses the hwloc [7] library to query the hardware hierarchy and builds internal hierarchical MPI communicators for each level at run-time. The unstructured mesh is input as distributed chunks which can be partitioned in any of the hierarchical levels by simply specifying one.

At present the library takes a top-down approach to hierarchical mesh partitioning [31] i.e., the partitioning starts at the highest level and cascades to the lowest hierarchical level. In a bottom-up approach [28] the application data is partitioned at the lowest hierarchical level and cascades up to map optimally onto the higher hierarchies. This results in a well balanced communication load but to construct the lowest level sub-domains a bootstrapping process using a top-down partitioner is necessary. Ideally a hierarchical mesh partitioning tool must support both paradigms.

4.1 Hardware topology builder

To understand the structure of the MPI tree topology built by TreePart one must understand few terminologies. Nodes are the individual computing units connected by a common network to create a computing pool or cluster. Each node is made up of multiple computing units (CPU) called sockets sharing a common NUMA memory pool. Note that accelerators like GPGPUs can also be included as additional sockets to the given node. A socket comprises of multiple cores that can simultaneously execute instructions. An example architecture and its topology is shown in figure 9. For the three level hierarchy shown in figure 10 we create three MPI communicators, namely node, socket, and core communicator. Except for the node communicator, the socket and core are local to a node.

Now we define two types of hierarchical communication called the (i) aggregation and (ii) cascade. In an aggregation process, data in a bottom level hierarchy is aggregated and moved to a top level one and cascade does just the opposite. Both operations are highly scalable because it does not involve network traffic across a node (always within the shared memory node). The data used for the aggregation or cascade is called the payload. Any operations across a node is only performed at the top-most level. This way we can control or restrict the number of ranks that participate in global communications to avoid network traffic. In fact nodes can be further aggregated based on their proximity to a network switch using the netloc library [16] but we post-pone this study as a future extension to TreePart.

Figure 9: (i) Topology of a node with one socket and two core with shared memory and individual/shared caches (left) (ii) Topology of four nodes on a network

Figure 10: Aggregate and cascade operations on a node with two multi-core sockets (payload is denoted by the coloured boxes)
4.2 One-sided distributed dictionaries

An integral part of TreePart is the one-sided distributed dictionary (ODD) data-structure. ODD is used to store unstructured mesh entities like nodes, elements, boundary faces, etc., as key-value pairs and perform scalable range queries on keys. The directory consists of arrays of key-value pairs distributed across any one of the hierarchical levels. The keys are of integral types and the values can be plain-old-data (POD) or variable length vectors (unlike ZoltanDD [13]). This assumption enables us to store the data already in a packed format in the directory structure for transmission. We use the assumed partitioning [2] method of Falgout et al. to initially distribute the keys globally and to perform scalable range queries on keys. During the rendezvous phase to determine the neighbours we use a blind send (or receive) query using one-sided MPI primitives, which is explained in detail in the following subsection. In current version of TreePart we assume that the level which initiates the queries to the ODD is at the same level as the ODD itself. Therefore the user is responsible for aggregating/cascading queries from a different level. But we plan to remove such restrictions in a future version.

4.3 Scalable blind send (or receive) queries

The blind send (or receive) problem can be described as follows. A set of MPI ranks called the blind initiator intends to send (or receive) data to (or from) its neighbouring MPI rank. The neighbouring rank (referred to as the blind end) is unaware of the fact that it must cooperate with the receiving (or sending) act. Usually an all-to-all type MPI primitive is used to transpose the send (or receive) matrix and obtain this information. We propose a scalable approach using one-sided accumulate primitive. Firstly we create an MPI window to expose an increment variable initialised to zero. Then the blind initiator calls an one-sided accumulate to its blind end variable which increments the value by one. Once all blind initiator have completed the accumulation; the blind end will have the number of ranks it is expected to cooperate with. A pseudo-code in C++ is provided in listing 1.

```cpp
int BlindCount(list<int> &rank_list) {
    int count = 0;
    int increment = 1;
    MPI_Win count_win;
    MPI_Win_create(&count, sizeof(int), 1, MPI_INFO_NULL, MPI_COMM_WORLD, &count_win);
    MPI_Win_fence(0, count_win);
    for (auto rank : rank_list) {
        MPI_Accumulate(&increment, 1, MPI_INT, MPI_SUM, count_win);
        MPI_Win_fence(0, count_win);
    }
    MPI_Win_free(&count_win);
    return count;
}
```

Listing 1: Counting blind send (or receive) C++ pseudo-code

This minimal information is sufficient to receive the data from all blind initiator of a blind end by probing for the message size using MPI_ANY_SOURCE (and MPI_ANY_TAG), allocating the buffers and finally completing the send or receive request. A brief pseudo-code in C++ is provided in listing 2.

```cpp
for (int i = 0; i < count; ++i) {
   // Do a receive or send
   MPI_Probe(MPI_ANY_SOURCE, MPI_ANY_TAG, MPI_COMM_WORLD, &stat);
   MPI_Get_count(&stat, MPI_BYTE, &size_in_bytes);
   // Allocate buffer using size
   ... 
   // Receive or send
   MPI_Recv(&buffer, size_in_bytes, MPI_BYTE, MPI_ANY_SOURCE, stat(MPI_SOURCE, stat(MPI_TAG, MPI_COMM_WORLD, &stat));
}
```

Listing 2: Blind communication (C++ pseudo-code)

The blind send combined with the assumed partition algorithm is a highly scalable infrastructure for ODD queries and we fully avoid the use of the inefficient all-to-all type primitives. In addition, we use ODD and blind communication to avoid Allgather type MPI operations to construct the dual graph of the mesh necessary for partitioning the mesh cells using graph partitioning libraries.

4.4 Hierarchical partitioning

TreePart currently implements a top-down hierarchical partitioning approach. The partitioning therefore starts at the top most level of the topology referred to as the bootstrap partition level (BPL). To start the process at BPL one first requires an approximately partitioned mesh available at this level (see figure 11). The payload can be positioned in any arbitrary level (usually the bottom-most level) and one has to aggregate the payload to the BPL. Then based on the users input the particular partitioning scheme is chosen and the mesh is redistributed based on the new partitioning. An illustration of this process is shown at the top of figure 11. Once the BPL partitions are obtained there are two ways the partitioning can proceed, (1) cascade equal mesh chunks to the next level and perform distributed parallel partitioning or (2) perform a shared-memory parallel partitioning in the current level and cascade partitions to the next level. An illustration of both approaches is shown in figure 11. Approach 2 is attractive because we completely avoid MPI communication and it also blends well with hybrid programming models. The partitioner terminates upon reaching the last level. We provide two ways to interface the unstructured mesh data to TreePart. In the library approach the mesh is assumed to be already divided (although not optimally) among all the participating ranks (lowest level) and supplied to TreePart using a ParMETIS style

![Figure 11: Bootstrap partition and approaches (1) and (2) to hierarchical partitioning considering two level node-socket hierarchy](image-url)
API function call to generate a refined partition. The mesh data is aggregated to BPL to start the partitioning process. In the second approach we provide a standalone tool which can read two popular formats CGNS unstructured mesh (experimental) and our in-house HiP HDF5 unstructured mesh format. The user executes the tool to generate HDF5 partition mesh files that can be read later for further processing.

4.5 ShHalo framework for shared-memory halo communication

MPI implementation that do not support kernel direct copy result in inefficient intranode communication. We encounter such situations quite often in practice. To handle such situations TreePart provides ShHalo, which is an MPI3 shared-memory optimised halo communication module. ShHalo wraps the original MPI calls for halo data communication and segregates them into inter and intranode communicators. The internode requests are initiated using network send and receive primitives. For intranode requests the data is copied directly to the neighbouring processor receive halo buffers using MPI3 shared-memory primitives as shown in figure 12. The users has to provide the halo communication schedule to aid ShHalo to pre-allocate the shared-memory buffers. Note that MPI3 shared-memory requires the use of its own allocation routines. Therefore one extra receive buffer is allocated for every halo entity. This approach requires minimal modification to the existing halo transfer in order to use ShHalo. A more intrusive approach is to get rid of halo intranode halo buffers in the users code and directly expose the neighbouring intranode processor’s memory. So the intranode transfer becomes simple direct memory-to-memory copy of halo data without any intermediate buffers (zero-copy ) [5].

4.6 Hierarchical load-balancing

Hierarchical load-balancing is the most distinguishing feature of TreePart. We have implemented mesh re-balancing using nodal and element weights that can work at any given hierarchical level. This gives the user the advantage of using the fast and scalable partitioning at the lowest level more frequently. TreePart uses shared-memory parallel partitioning at lower levels thus totally avoiding MPI communications as shown in figure 13. The re-balancing cost is drastically reduced since we restrict the movement of data within the node. The expensive node level re-balancing of the mesh can be called less frequently to considerably reduce the re-balancing cost. The user can optimise the re-balancing frequency across levels for his application to achieve significant reductions in run-time.

5 RESULTS

We interfaced TreePart library with our in-house solver AVBP using the ParMETIS style API of TreePart. We study the deflagrating flames of compressed natural gas (CNG) [26] using large eddy simulation (LES) with a two step reaction model. The computational domain is an unstructured mesh with 150M tetrahedral elements. The transient, turbulent flame fronts that propagate past a sequence of solid obstacles, whose geometry and computational domain is shown in figure 14. The chamber is square in cross-section with internal dimensions of length, 250 mm and side, 50 mm producing an overall volume of 0.625 l and a length to width ratio of 5. The arrow in figure 14 indicates the direction of the flame propagation.
5.1 Solver scalability with hierarchical partitioning

The strong scalability results of the combustion test case using online hierarchical partitioning for different MPI rank counts (\(\#\) of partitions) is shown in figure 15. Note that ParMETIS failed to generate online partitions for this test case beyond 2k MPI ranks and PT-SCOTCH failed beyond 5k but the hierarchical partitioner successfully generated partitions online beyond 25k MPI ranks. The plain graph partitioners failed due to MPI exit errors in the all-to-all function.

5.2 Effect of processor placement and intranode communication

Hierarchical partitioning places MPI ranks efficiently on to processor cores and avoids unnecessary inter node communication. In addition ShHalo MPI3 shared memory optimisation can be applied to further optimise intranode halo data communication. To show the effect of processor placement and the ShHalo optimisation we ran four test cases with different partitioning scheme, (1) plain non-hierarchical parallel graph partitioning, (2) plain non-hierarchical geometric recursive coordinate bisection (RCB) without ShHalo, and (4) topology-aware hierarchical RCM with ShHalo optimisation. Note that the RCB partitioner gives lower quality partitioning compared to a graph based partitioner because it does not consider edge-cut information. On the contrary it produces almost perfectly balanced partitions compared to graph. We ran the cases on 10 nodes, where each node consists of two sockets of 18 core Intel Xeon processor. This brings the total core count to 360.

The solver time taken per iteration is plotted in figure 16 for the four test cases. As mentioned previously the plain RCB partitioner results are worse than the plain graph partitioner. We see that by placing the partitions correctly using topology-awareness RCB is more efficient than the plain graph partitioner. With the shared-memory optimisation we see even further speed up.

5.3 Effect of hierarchical load-balancing

To load-balance the mesh we require to calculate weights of the mesh entities based on runtime timing measurements. The measurement must not be too coarse grained otherwise we risk averaging out important deviations in runtime that requires balancing. Our solver already employs an optimisation to improve cache utilisation by dividing mesh elements into cache block groups (see figure 8). Therefore we measured the computational time of each cache block and spread this value to the elements in the block by dividing by the total number of elements in the block. This way we minimise the risk of using a very coarse grain timing and at the same time avoid the risk of getting erroneous measurements by going too fine grain. The improvement in load balance before and after performing one iteration of TreePart hierarchical load-balancing at the two bottom-most levels (2 sockets and 24 cores) is shown in figure 17. The case was run on 10 nodes with 2 sockets having 24 cores each. Even with a coarse grain timing information and load-balancing across the lowest two levels considerable improvement in load balance is achieved and the reduction in computational time per solver iteration is shown in figure 17.

5.4 Comparison of load-balancing timing across hierarchy

The cost of load-balancing should be as low as possible so that it does not shadow the actual gain in computational speedup as a result of the load-balancing. A hierarchical load-balancing algorithm enables one to load-balance fine grain partitions at the lowest level more frequently than higher levels. Thus providing more flexibility in optimising the load-balancing frequency. In figure 18 we compare the repartitioning time between different hierarchical levels, flat partitioning considering all 480 ranks and gain in solver time per iteration due to partitioning across shared memory levels (1 and 2). Firstly we notice that the bootstrap partitioning time is much higher than the cost of a flat partitioning considering no hierarchy. This is mainly because the RCB used is a pure MPI implementation and does not exploit the shared memory cores available at the bootstrap level. Using a hybrid parallel RCB algorithm will considerably bring down the repartitioning cost at the bootstrap level. This also provides an interesting use case for hybrid parallel graph partitioning algorithms. The cost of repartitioning at levels L1 and L2 are considerably lower than the flat partition. Moreover repartitioning
Table 1

| Partition Type       | Partition Time (s) | Solver Time (s) | Reduction due to LB on L2 (s) |
|----------------------|--------------------|-----------------|------------------------------|
| Bootstrap partition  | 8,117              | 95             | 0                            |

![Figure 17: Mean normalised time of each partition before and after load-balancing considering 2 sockets of 24 cores across the 10 bootstrap nodes each with 2 sockets (level 1) of 24 cores (level 2) i.e., 10 x 2 x 24 hierarchy](image)

![Figure 18: Comparison of load-balancing time across hierarchy of 10 bootstrap nodes each with 2 sockets (level 1) and 24 cores (level 2) i.e., 10 x 2 x 24 hierarchy](image)

at level 1 or 2 does not involve communication across the network and highly local. The gain in speed-up due to repartitioning at level 1 and 2 is easily amortized by the gain in computational time gained per iteration. The focus of the present work is the demonstration of TreePart and its hierarchical load-balancing ability. Therefore we postpone the study on the actual optimisation of the solver and TreePart hierarchical load-balancing to as an extension of the present work.

6 FUTURE WORK

Parallel distributed breadth first search algorithm (BFS) [8] is useful to find connected components in a graph. Such a BFS implementation in TreePart can be used to ensure connected partitions because distributed graph partitions can produce disconnected ones. Disconnected partitions are undesirable for test cases involving Lagrangian particle dynamics, parallel mesh adaptation, etc. The BFS will be used to merge the disconnected mesh entities by re-migrating to the correct connected rank. We are making TreePart more HPC aware by interfacing with netloc [16] library to build network awareness; map ranks optimally by exploiting network proximity information. Currently the hierarchical framework supports only single weights. Implementing multiple weights for load-balancing is planned. Hierarchical techniques in TreePart are quite attractive to parallel mesh adaptation implementation, which we plan as a future extension. Finally we plan to release TreePart as open-source software for benefit of the HPC community.

7 CONCLUSION

With the advent of advanced features and optimisations like MPI3 shared-memory, HPC awareness, etc., the performance issues in plain MPI codes even for very large number of ranks can be made competitive to hybrid MPI implementations. This approach has an advantage of introducing minimal changes to HPC codes to achieve the said performance. The critical issues that we identified that hinder the performance of plain MPI codes are (i) load balancing, (ii) minimising redundant computation at halo entities and (iii) reliable partitioning of meshes into extremely high partition counts in HPC codes. We have developed the TreePart library to address these problems using a variety of optimisations resting on the core principle of hardware-awareness and scalability. We showed excellent improvement in our industry strength and highly optimised in-house combustion LES code using TreePart. We hope that plain MPI HPC codes using TreePart is a viable alternative and also a companion to hybrid MPI counterparts.

REFERENCES

[1] Yaroslav Akhremtsev, Peter Sanders, and Christian Schulz. 2015. (Semi-)External Algorithms for Graph Partitioning and Clustering. In 2015 Proceedings of the Seventeenth Workshop on Algorithm Engineering and Experiments (ALENEX). Society for Industrial and Applied Mathematics, Philadelphia, PA, 33–43. https://doi.org/10.1137/1.97816119735744

[2] A. H. Baker, R. D. Falgout, and U. M. Yang. 2006. An assumed partition algorithm for determining processor inter-communication. Parallel Comput. 32, 5-6 (Jun 2006), 394–414. https://doi.org/10.1016/j.parco.2006.06.009

[3] Pavan Balaji, Darius Buntinas, David Goodell, William Gropp, Torsten Hoefler, Sameer Kumar, Ewing Lusk, Rajeev Thakur, and Jesper Larsson Traff. 2011. MPI on millions of cores. Parallel Processing Letters (2011). https://doi.org/10.1142/ S012962641100060

[4] Gilad Ben-Yossef. 2009. On Threads, Processes and Co-Processes. In CELF CELF Embedded Linux Conference Europe. Grenoble.

ACKNOWLEDGMENTS

The research leading to these results has received funding from the European Union’s Horizon 2020 research and innovation programme under the EPEEC project, grant agreement No 801051. This work was granted access to the HPC resources of IDRIS under an allocation by GENCI for the Grand Challenges Jean Zay (2019).
Jean-Baptiste Besnard, Allen Malony, Sameer Shende, Marc Pérache, Patrick Carribault, and Julian Jaeger. 2015. An MPI Halo-Cell Implementation for Zero-Copy Abstraction. In Proceedings of the 22nd European MPI Users’ Group Meeting on ZZZ – EuroMPP 15. ACM Press, New York, New York, USA, 1–9. https://doi.org/10.1145/2802658.2802669

Erik G. Boman, Umit V. Çatalyürek, Cédric Chevalier, and Karen D. Devine. 2012. The Zoltan and Torporia parallel toolkits for combinatorial scientific computing: Partitioning, ordering and coloring. Scientific Programming (2012). https://doi.org/10.3233/SPR-2012-0342

François Bocko, Jérôme Côté-Ortega, Stéphanie Moreourd, Nathalie Furmento, Bruce Goglin, Guillaume Mercier, Samuel Thibault, and Raymond Namyst. 2010. bwloc: A generic framework for managing hardware affinities in HPC applications. In Proceedings of the 18th Euromicro Conference on Parallel, Distributed and Network-Based Processing, PDP 2010. https://doi.org/10.1109/PDP.2010.67

Aydin Buluç and Kamesh Madduri. 2008. PT-Scotch: A tool for efficient parallel graph ordering. Parallel Computing. (2008). https://doi.org/10.1016/j.parco.2007.12.001 arXiv:0907.1375

K. Devine, E. Boman, R. Heaphy, B. Hendrickson, and C. Vaughan. 2002. Zoltan and the chapel language. International Journal of High Performance Computing Applications. (2002). https://doi.org/10.1109/5992.988653

Craig C. Douglas, Jonathan Hu, Markus Kowarschik, Ulrich Rude, and Christian Weiss. 2000. Cache optimization for structured and unstructured grid multigrid. Electronic Transactions on Numerical Analysis. (2000).

Assafad Hadiid Gehremedhin, Frederic Manne, and Alex Pothen. 2005. What Large-Scale Numerical Simulations. In 2018 IEEE/ACM 9th Workshop on Latest Advances in Scalable Algorithms for Large-Scale Systems (scAlA). IEEE, 65–72. https://doi.org/10.1109/ScAlA.2018.806012

A. R. Maati, A. Allbari, S. Meares, and S. S. Ibrahim. 2012. A Comparative Study of Turbulent Premixed Flames Propagating Past Repeated Obstacles. Industrial & Engineering Chemistry Research 51, 22 (jun 2012), 7690–7703. https://doi.org/10.1021/ie201928q

John Mellor-Crummey, David Whalley, and Ken Kennedy. 2001. Improving memory hierarchy performance for irregular applications using data and computation reorderings. International Journal of Parallel Programming (2001). https://doi.org/10.1016/1073-5869(98)00041-2

Vincent Moureau, Pascale Domingo, and Luc Vervisch. 2011. Design of a massively parallel CFD code for complex geometries. Comptes Rendus Mécanique 339, 2–3 (feb 2011), 141–148. https://doi.org/10.1016/j.crme.2010.12.001

M. Pawankumar and K. N. Kausahil. 2013. Revisiting the space-filling curves for storage, reordering and partitioning mesh based data in scientific computing. In 20th Annual International Conference on High Performance Computing, HPC 2013. https://doi.org/10.1109/HPC.2013.6799697

Rolf Rabenseifner. 2003. Hybrid Parallel Programming on HPC Platforms. 5th European Workshop on OpenMP (2003).

Rolf Rabenseifner, Georg Hager, and Gabriele Jost. 2013. Hybrid MPI and OpenMP Parallel Programming MPI + OpenMP and other models on clusters of SMP nodes. Tutorial at ICS at SC 2013. 427–436.

Ken Rafteri, Abdelhelam Amer, Lena Oden, Charles Archer, Wesley Bland, Hajime Fujita, Yanfei Guo, Tomislav Janjicue, Dmitry Durnov, Michael Blackcombe, Min Si, Sangmin Seo, Akhil Langer, Gengbin Zheng, Masamichi Takagi, Paul Colman, Jithin Jose, Sayantan Sun, Alexander Sannikov, Sergey Oblomov, Michael Chuvilev, Masayuki Hatanaka, Xin Zhao, Paul Fischer, Thilina Rathnayake, Matt Otten, Misun Min, and Pavan Balaji. 2017. Why is MPI so slow? Analyzing the fundamental limits in implementing MPI-3. In Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis, SC 2017. https://doi.org/10.1145/3126908.3126963

Mohammad Javad Rashidi, Jonathan Green, Pavane Balaji, Ahmad Afshahi, and William Gropp. 2011. Multi-core and network aware MPI topology functions. In Lecture Notes in Computer Science (including subseries Lecture Notes in Artificial Intelligence and Lecture Notes in Bioinformatics). https://doi.org/10.1007/978-3-642-44449-0_8

Sasko Ristov, Radu Prodan, Marjan Gusev, and Karolj Skala. 2016. Superlinear speedup in HPC systems: Why and when?. In Proceedings of the 2016 Federated Conference on Computer Science and Information Systems, FedCSIS 2016. https://doi.org/10.15439/2016F498

Thilo Schonfeld and Michael Rudgward. 1999. Steady and unsteady flow simulations using the hybrid flow solver AVBP. AIAA journal 37, 11 (1999), 1375–1385.

Christian Schulz, Jesper Larsson Traff, and Konrad von Kirchbach. 2017. Better Process Mapping and Sparse Quadratic Assignment. (feb 2017). arXiv:1702.04164 http://arxiv.org/abs/1702.04164

Andre Silva, Rafael Bohrer Aval, Marcos Ennes Barreto, and Philippe Olivier Alexandre. 2000. DPC++: Object-Oriented Programming Applied to Cluster Computing. In PDPTA.

J.D. Terecs, J. Falk, and J.E. Flaherty. 2005. Resource-Aware Scientific Computation on a Heterogeneous Cluster. Computing in Science and Engineering 7, 2 (mar 2005), 40–50. https://doi.org/10.1109/MCSE.2005.38

R. Thakur, P. Balaji, D. Buntinas, D. Goodell, W. Gropp, T. Hoefler, S. Kumar, E. Lusk, and J. L. Tratt. 2010. MPI at Exascale. Proceedings of SciDAC (2010).

Miao Wang, Yuhua Tang, Xiaowei Guo, and Xiaoguang Ben. 2012. Performance analysis of the graph-partitioning algorithms used in OpenFOAM. In 2012 IEEE 5th International Conference on Advanced Computational Intelligence, ICACI 2012. https://doi.org/10.1109/ICACI.2012.663129

Sam White and Laxmikant V. Kale. 2018. Optimizing point-to-point communication between adaptive MPI endpoints in shared memory. https://doi.org/10.1002/cpe.4467