Effective implementation of the High Performance Conjugate Gradient benchmark on GraphBLAS

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Abstract—Applications in High-Performance Computing (HPC) environments face challenges due to increasing complexity. Among them, the increasing usage of sparse data pushes the limits of data structures and programming models and hampers the efficient usage of existing, highly parallel hardware. The GraphBLAS specification tackles these challenges by proposing a set of data containers and primitives, coupled with a semantics based on abstract algebraic concepts: this allows multiple applications on sparse data to be described with a small set of primitives and benefit from the many optimizations of a compile-time-known algebraic specification. Among HPC applications, the High Performance Conjugate Gradient (HPCG) benchmark is an important representative of a large body of sparse workloads, and its structure poses several programmability and performance challenges. This work tackles them by proposing and evaluating an implementation on GraphBLAS of HPCG, highlighting the main changes to its kernels. The results for shared memory systems outperforms the reference, while results in distributed systems highlight fundamental limitations of GraphBLAS-compliant implementations, which suggests several future directions.

Index Terms-hpcg,multigrid,red-black gauss-seidel,graphblas

I. INTRODUCTION

The High-Performance Computing (HPC) landscape is currently facing challenges due to the steadily increasing complexity of applications and platforms. Applications from both classical scientific domains like physics and newer domains like data analytics or Artificial Intelligence (AI) require attaining high performance metrics while at the same time keeping programming efforts under control. An important trend is the adoption of sparse data, which model some real-world scenarios where certain entities are associated to others and only a small subsets of all possible associations is of interest. Examples of this trend are diverse, ranging from Finite Elements Methods (FEMs)-based applications for physics [1] to graph-based applications for the analysis of large data sets [2]. Computing platforms are also becoming increasingly complex, and writing reliable and performing applications requires nowadays costly expertise and platformspecific tools. Current software solutions also fall short in adapting to the growing landscape of HPC applications while ensuring effective hardware usage.

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In this scenario, applications of special interest in HPC are iterative solvers for sparse linear systems [3], which allow studying many physical problems by relying on a sparse description of the physical system. Several software packages implement sparse solvers on different hardware platforms [4], and the research is increasingly active. As a consequence, the need for standardization and comparison led to the introduction of a widely-accepted HPC benchmark named High Performance Conjugate Gradient (HPCG) [5], from which the eponymous HPCG rank for supercomputers was created [6]. HPCG solves a sparse linear problem Ax = b, where A is a sparse matrix of size $n \times n$, b a dense, known vector and x the unknown vector. Unlike dense solvers such as the wellknown High Performance Linpack (HPL) suite [7], HPCG fully exploits the sparsity of the A matrix by implementing an iterative solver algorithm whose time and space complexity are proportional to the number of non-zeroes in A and by using suitable data structures. Although HPCG solves a specific physical problem, the algorithms it is composed of represent a wide class of solvers, and the ranking guidelines disallow problem-specific optimizations [8].

Despite standardization efforts, multiple data structures for sparse data exist, whose choice depends on various factors (sparsity pattern, computation, hardware, etc.); as a consequence, the implementation of algorithms may strongly vary, leading to a complex design space. Instead, productivity calls for an abstract representation of the computation as close as possible to its algebraic formulation: this led to the introduction of GraphBLAS [9], a specification to develop algorithms for graphs with strong algebraic foundations. Unlike BLAS [10] and other frameworks, GraphBLAS does not prescribe a specific storage format for vectors and matrices, leaving the choice to the specific implementation. This abstraction enables domain experts to develop algorithms that are portable and leave optimizations to the specific implementation, thus achieving a complete separation of concerns.

Despite the increasing adoption of GraphBLAS, sparse solvers are still an area of active development and challenge both the GraphBLAS specification and its implementations. This paper presents an implementation of HPCG on top of GraphBLAS, addressing the related design and implementation choices. Hence, it brings the following contributions:

- it discusses the main design decisions to implement HPCG on top of GraphBLAS, showing how its kernels can be implemented on top of opaque data structures
- it assesses the performance of the implementation in shared memory systems typical of HPC environments, outperforming the reference with no manual or architecture-specific optimization efforts
- it assesses the performance of the implementation in a distributed system, showing current limitations
- it discusses theoretical limitations and possible advancements to the current implementations and to the Graph-**BLAS** specification

This paper is organized as follows. Section II introduces to the background information, in particular the problem HPCG solves, its main kernels and the GraphBLAS specification. Section III discusses the design decisions necessary to implement HPCG on top of GraphBLAS. Section IV explains the main characteristics of the implementation, while Section V shows its evaluation on several HPC-grade systems. Section VI highlights the main efforts to accelerate HPCG on HPC architectures. Finally, Section VII discusses the achievements of this work and possible future work.

II. BACKGROUND

This section explains the structure of the HPCG benchmark, its kernels and performance characteristics. It then describes the aspects of GraphBLAS that are relevant to this paper.

A. The HPCG benchmark

Many problems of interest to physicists and engineers are represented by Partial Differential Equationss (PDEs) and model the problem space as a 1D, 2D or 3D grid. Elliptic PDEs are an important class, as they describe many common problems and are usually discretized on a 3D spatial grid of $n_x \times n_y \times n_z = n$ points, where the interactions are modeled according to the physics of the system. These interactions often involve only points that are spatially close (e.g., within a halo), producing inherently sparse matrices.

HPCG [8, 11] solves a heat-diffusion problem on a semiregular 3D grid via a preconditioned Conjugate Gradient (CG) solver [12], modeling heat exchanges among neighboring elements. HPCG main kernels are:

- 1) input generation
- 2) Conjugate Gradient solver, in turn relying on the
- 3) Multigrid preconditioner, implemented on top of the
- 4) Symmetric Gauss-Seidel smoother;
- 5) restriction and refinement, to recursively call the Multigrid (MG) preconditioner and use its result;

The following sections delve into the details of these kernels.

B. Input generation

An iterative sparse solver has three inputs: the system matrix A, the right-hand side vector b and the initial hint for the solution $x^{(0)}$. Since HPCG simulates a well-known heat diffusion problem on a semi-regular grid, these inputs are generated automatically, with b = 1 and $x^{(0)} = 0$.

Listing 1: Steps of the MG preconditioner

```
function MG(mg_level, z, r)
 2
         z \leftarrow \text{sgs\_smoother}(\text{mg\_level}, z, r)
 3
         if (mg_level.coarser_sys = nil)
 4
            return z
 5
         f \leftarrow mg\_level.A * z
         r_c \leftarrow \text{restrict}(\text{mg_level}, r - f)
 6
 7
         z_c \leftarrow 0
 8
         z_c \leftarrow MG(mg\_level.coarser\_level, z_c, r_c)
 9
         z \leftarrow z + \text{refine}(\text{mg_level}, z_c)
10
         z \leftarrow \text{sgs\_smoother}(\text{mg\_level}, z, r)
```

```
11
      return z
```

1

C. Conjugate Gradient solver

The CG solver [12] is a generic, iterative algorithm for the solution of PDEs, which starts from the user-given solution $x^{(0)}$ and iteratively refines it until converging to the final solution $x^{(i)}$ after *i* iterations, or until the solution is "close enough", i.e., until the module of the residual vector $r = b - Ax^{(i)}$ is smaller than a given threshold. The main computational kernels of CG are the sparse vector product spmv, the dot product of two vectors dot and the linear combination of two vectors waxpby. Among them, spmv dominates the runtime due to its complexity: HPCG system matrix A, which represents a semi-regular 3D grid with halo 1, has from 8 to 27 nozeroes per rows, resulting in a total size $\Theta(n)$. Therefore, the work complexity of an spmv operation in HPCG, and thus of an iteration of the CG solver, is $\Theta(n)$.

D. Multigrid (MG) preconditioner

The second main kernel of HPCG is the MG preconditioner [13], which improves the convergence towards the solution at the cost of higher complexity and slightly less generalization w.r.t. the CG solver. This preconditioner improves the initial solution by computing an approximation z of $A^{-1}r$ in a recursive fashion, which then contributes to the main solution of CG $x^{(i)}$. It does so by attempting to solve a problem Az = rthrough successive, recursive restriction and refinement steps: on each recursion the current solution z (initially 0) is improved by a smoothing step and by solving a smaller problem based on a restriction of r and z; the result of this recursive problem is then refined and contributed back to z.

Listing 1 sketches the MG preconditioner in more detail:

- 1) line 2: smooth z from r via the Symmetric Gauss-Seidel (SGS) smoother, so that $Az \approx r$;
- 2) lines 3-4: if the maximum number of coarsening levels has been reached, simply return the current solution z;
- 3) line 5: compute $f \leftarrow Az$, i.e., the current residual for the problem Az = r;
- 4) line 5: compute the restricted residual r_c for the problem Az = r, i.e., the restriction of r - f;
- 5) line 8: improve the initial $z_c \leftarrow 0$ (line 6) by recursively calling the MG preconditioner on r_c and the coarser system *mg_level.coarser_level*;
- **line 9**: refine z_c to the current system and add it to z_c 6) thus improving on the initial solution z;

7) **line 10**: smooth *z* again to remove oscillatory components added in the previous step.

E. Symmetric Gauss-Seidel (SGS) smoother

The basic Gauss-Seidel (GS) algorithm smooths z by updating each value z_i of it as

$$z_i \leftarrow (A_{i,i})^{-1} \left(r_i - \sum_{j=0, j \neq i}^{n-1} A_{i,j} z_j \right) \quad 0 \le i < n; \quad (1)$$

essentially, Equation (1) solves the *i*-th equation of the problem Az = r. GS prescribes the order of increasing *i* to compute Equation (1), causing the output value z_i to depend on the input values z_j , j < i computed in the previous iterations of Equation (1) and for which $A_{i,j} \neq 0$; hence, $A_{i,j} \neq 0$ determines the presence of direct (i, j) dependencies, which then propagate transitively across values depending on A. Therefore, the available parallelism depends on A itself. For HPCG, A is a semi-regular grid over a homogeneous spatial domain, which causes (i, j) dependencies to propagate transitively from all j < i, making the execution of GS in HPCG inherently sequential, a major performance bottleneck in HPC highly parallel systems.

The SGS version adds to the previous step (called *forward sweep*) another step, called *backward sweep*, which performs the same operations but with *i* from n - 1 to 0, improving the convergence for many problems [13]; nonetheless, the aforementioned performance issue holds for SGS as well.

The complexity of SGS in HPCG also depends on the structure of A, because Equation (1) is computed n times for each row i of A. Since each row has $\Theta(1)$ nozeroes, the total work complexity of SGS is $\Theta(n)$.

F. Restriction and refinement

The restriction operation projects a vector from a fine space to a coarse space, the refinement operation does the opposite. Restriction occurs to create the inputs for the coarser problem (line 6 of Listing 1), whose output is refined to improve the current solution (line 9).

HPCG restriction operation implements *straight injection* [14]: it restricts the vector in the fine space by a factor of two along each dimension and populates each point of the coarse vector with the value at the lowest coordinates of the corresponding octet in the fine space. Correspondingly, the refinement operation populates the finer vector with the corresponding values of the coarse vector and zeroes elsewhere.

As these operations move data in a fixed sparse pattern and do not require computation, the HPCG reference implementation performs it *in-place* by directly accessing the input and output arrays, thus making assumptions on the data structure.

HPCG 3D input domain requires restricting/refining vectors by a factor eight; furthermore, the number of restriction/refinement levels is limited to a fixed number (typically 4), for a total work complexity of $\Theta(n)$. Hence, the whole work complexity of HPCG reference implementation is $\Theta(n)$.

G. Data distribution for distributed execution

A focal design aspect of the reference HPCG implementation is the data distribution across nodes for distributed execution. To achieve minimal data exchange, the reference optimally splits the physical simulation grid of sizes $n_x \times n_y \times n_z = n$ across the p nodes. To achieve optimality, it computes the factorization $p = p_x \times p_y \times p_z$ that maps optimally to the $n_x \times n_y \times n_z$ grid. In this way only the 2D halos in the physical space need to be exchanged among nodes: if each local dimension is $s_d = n_d/p_d$, $d \in \{x, y, z\}$, the number of points each node exchanges with its eight 3D neighbors is $h = 2(s_x s_y + s_y s_z + s_x s_z)$. The rows of matrix A are partitioned following this distribution and nodes update only vector data during the computation. Hence, if $n_d = \Theta(\sqrt[3]{n})$ and $p_d = \Theta(\sqrt[3]{n^2/p^2})$ values before an mxv operation.

H. The GraphBLAS specification and its implementations

GraphBLAS [9] is a specification based on two core concepts: graphs can be represented via matrices and algorithms on graphs can be expressed via algebraic operations defined over algebraic structures like monoids and semirings. These abstractions ease programming while providing with solid assumptions to carry optimizations, like the properties of the algebraic structure. This specification stresses the importance of sparse data structures and operations, and is thus a good fit for modern HPC applications and for sparse linear solvers in particular, inasmuch it allows domain experts to implement algorithms without extensive programming and optimization efforts, while ensuring good performance thanks to its performance semantics. From a high-level perspective, a GraphBLAS program is thus a sequence of standard algebraic operations like spmv, dot and waxpby performed on opaque data structures representing matrices and vectors, augmented with information about the algebraic structure.

Containers opaqueness allows implementations the freedom to make different choices based on the platform and the data, which determines performance. Multiple implementations of the official C specification [15] exist, like Suit-Sparse:GraphBLAS [16], vendor-specific ones [17] and also C++ implementations [18, 19], which employ template metaprogramming to optimize operations based on the user-given algebraic structure.

III. DESIGN OF HPCG KERNELS FOR GRAPHBLAS

This section explains the design decisions to implement HPCG on GraphBLAS. Some HPCG kernels in Section II-A require little effort, because the operations in GraphBLAS closely match those in the reference HPCG implementation. This is the case for the CG solver, which is composed of standard algebraic operations that easily map to GraphBLAS, keeping the same work complexity $\Theta(n)$ of the reference. Instead, the components of the MG preconditioner do not straightforwardly map. The following sections explain their design.

Listing 2: GraphBLAS pseudo-code for the RBGS forward pass

```
function grb_rbgs_forward(mg_level, z, r, c)
1
      for k from 0 to c
2
3
        s \leftarrow \max (\operatorname{mg_level.} colors[k])
4
           mg_level.A, z)
5
         apply (i -> \{z[i] \leftarrow (r[i] - s[i] +
6
              z[i] * mg_level.A_diag[i]) /
              mg\_level.A\_diag[i]},
7
8
              mq_level.colors[k])
9
      return z
```

A. Symmetric Gauss-Seidel (SGS) smoother

As from Section II-E, HPCG smoother is, in combination with its input, inherently sequential. Furthermore, the ordering of updates to z_i in Equation (1) makes this kernel not easily expressible with standard algebraic operations. One could attempt to workaround this latter limitation, e.g., by implementing the SGS kernel with n spmv operations on nvectors and updating one point at a time, but the time and memory overheads of such a solution would be prohibitive, and the execution would still be sequential.

Instead, multiple works [20, 21] replace the SGS smoother with Red-Black Gauss-Seidel (RBGS), which overcomes these limitations by relaxing some (i, j) dependencies via a partitioning scheme that groups together indices. Indeed, HPCG technical specification [8] allows changing the smoother under the condition that the new one passes the internal symmetry test. RBGS relaxation enables updating independent indices in parallel at the cost of a higher number of iterations to achieve the same smoothing effect of GS [22]. Nonetheless, the performance gain thanks to parallelisation usually outweighs the higher number of iterations.

If the partitioning scheme finds c colors C_k , $0 \le k < c$, all z_i for which $i \in C_k$ can be updated in parallel as in Equation (1). This allows implementing RBGS with natively parallel GraphBLAS primitives, as Listing 2 sketches: here, operations on all elements of a color k are implemented with GraphBLAS primitives, thus inherently parallel; instead, colors are processed sequentially (loop of line 1) to meet the dependencies among them. The masked mxv of line 3 implements the summation of Equation (1) for all values of color k: the first argument mg_level.colors[k] is a binary mask marking the indices $i \in C_k$, so that mxv computes the outputs only for these positions into s. The following apply operation applies the lambda in the first argument in parallel for all marked elements of the mask, i.e., for all $i \in C_k$, computing the remaining part of Equation (1) and then updating z_i as a side effect. This function needs to access the diagonal value of A, which is stored in a dedicated vector mg_level. A_diag since GraphBLAS does not allow accessing individual matrix values in constant time. This vector is initialized during input generation.

An effective partitioning scheme depends on A: the larger the parts of a partitions, the larger the exposed parallelism. For HPCG, an effective and simple partitioning scheme can be implemented via a greedy coloring algorithm [23] that tracks only direct (i, j) dependencies: if there is a direct (i, j) dependence, than i and j must have different colors. Higher parallel efficiency is achieved when the number of colors is low, i.e., the coloring is near-optimal. For HPCG 3D grid, greedy coloring achieves optimal results, finding eight colors.

Partitioning schemes other than our greedy one are possible. Some of them also group the indices to improve the spatial locality of data accesses [20, 21], so that indices having the same color C_k are stored in physically contiguous positions. The choice of a more advanced partitioning scheme depends on the physical domain and is thus orthogonal to the programming framework, and hence outside the scope of this work. In the reference implementation, any grouping of indices can be realized by manipulating the data structures of the system A, which are non-opaque, while GraphBLAS makes this impossible because of containers opaqueness. However, a grouping scheme can be performed via a row *permutation* matrix P and its transposed P^T as $P^T AP$, which is supported in GraphBLAS via the mxm operation.

Since RBGS is a relaxation of GS to expose more parallelism, its work complexity also takes into account the number of processing units p. With serial execution the work complexity is still $\Theta(n)$, because it performs the same computation of Equation (1), though in a different order. Under the assumption that all partitions are large enough to efficiently parallelise their computation using p cores, the expected speedup is p. Since n is orders of magnitudes higher than p in realistic workloads and the coloring algorithm we use here can optimally identify the eight colors for HPCG input domain, we indeed assume this assumption holds and that RBGS has work complexity $\Theta(n/p)$.

B. Restriction and refinement

The HPCG reference implementation directly accesses the storage to compute both restriction and refinement, which is impossible in GraphBLAS because vectors are opaque objects. As HPCG *straight injection* restriction is a linear operation, it corresponds to a matrix-vector multiplication with a rectangular matrix of sizes $n \times \frac{n}{8}$ and naturally is expressible in GraphBLAS. Similarly, HPCG refinement is the transposed operation of restriction. Therefore, the work complexity is that of an mxv operation on HPCG, i.e., $\Theta(n)$.

This constraint forces the materialization of a matrix, whereas HPCG reference implements restriction as an array of indices to copy from the fine vector to the coarse one, and uses the same vector to implement refinement. Because of the data structures typically used to describe sparse matrices, e.g., the three arrays of Compressed Sparse Row (CRS) [24], a GraphBLAS implementation of refinement/restriction may incur additional storage and time overheads compared to the reference; the work complexity, however, is the same.

IV. IMPLEMENTATION

We implement HPCG on GraphBLAS using a C++ variant of the GraphBLAS specification by Yzelman et al. named

Listing 3: ALP/GraphBLAS C++ implementation of the forward RBGS pass. Error checking omitted.

```
void grb_rbgs_forward(
1
2
      const Matrix<double> &A,
 3
      const Vector<double> &A_diaq,
 4
      const std::vector<Vector<bool>> &colors,
 5
      const Vector<double> &r,
      Vector<double> &x,
 6
 7
      Vector<double> &tmp, // workspace buffer
 8
      Ring &ring
 9
   )
      {
      for(size_t c = 0;c < colors.size();++c) {</pre>
10
11
        mxv<descriptors::structural>(
          tmp, colors[c], A, x, ring);
12
        eWiseLambda( [&] (size_t i) {
13
14
            double d = A_diag[i];
            double v = r[i]-tmp[i]+x[i]*d;
15
            x[i] = v/d; \},
16
17
          colors[c], x, r, tmp, A_diag);
18
      }
    }
19
```

ALP/GraphBLAS [19], which describes GraphBLAS primitives and their algebraic structure via C++ templates to leverage the (algebraic) type safety checks and the automatic performance optimization of modern compilers via template meta programming- while keeping a concise code base. From here on, we call this implementation ALP. We expect ALP to attain performance comparable to that of a hand-coded C/C++ application such as the HPCG reference code, which is also coded in C++ that, similar to ALP/GraphBLAS, does not employ abstractions that may prevent compiler optimizations, thus enabling a fair comparison of the two implementations. Listing 3 implements the forward pass of RBGS with ALP/-GraphBLAS, showing in red and orange the GraphBLAS containers and primitives, respectively. It closely follows the structure of Listing 2, showing the A,A_diag,colors fields of mg_level in Listing 2 as explicit C++ function parameters: here, the color masks are passed via a common C++ data structure storing the boolean masks of type Vector<bool>.

ALP/GraphBLAS provides several *descriptors* to pass domain information to operations. In line 11 of Listing 3 ALP/-GraphBLAS *structural* descriptor leverages the optimized implementation of Vector for sparsity, causing mxv to ignore the actual nonzero value of the color mask colors[c] and follow only the sparsity pattern, avoiding useless memory accesses. Another example is the refinement operation of Section III-B, which uses the restriction matrix transposed; to avoid materializing the transposed matrix, the mxv operation for refinement is added the *transpose_matrix* descriptor to use the restriction matrix directly.

ALP/GraphBLAS also provides several *backends*, i.e. implementations of containers and operations tailored to different execution environments that can be chosen at compile time and that all meet GraphBLAS performance semantics. Throughout our experiments, ALP uses the *shared-memory* backend for multicore machines and the *hybrid* backend for distributed and

TABLE I: BSP asymptotic cost components for the distributed implementations.

	Ref	ALP
computation communication	$\frac{n/p}{\sqrt[3]{n^2/p^2}}$	$\frac{n/p}{n/p(p-1)} \approx n$
synchronization	1	1

multicore execution. The shared-memory backend distributes the execution among cores using OpenMP threads, taking into account Non Uniform Memory Access (NUMA) architectures via a NUMA-aware memory allocator [25] and preferring interleaved allocations to balance memory accesses among domains and avoid bottlenecks. The hybrid backend relies on the Lightweight Parallel Foundations (LPF) communication layer [26] to provide high-performance communication functionalities. The LPF interface and semantics abide by the Bulk-Synchronous Parallel (BSP) [27] model of computation, while the hybrid ALP/GraphBLAS backend assumes a 1D grid of nodes and splits matrix rows and vectors according a block-cyclic distribution. This requires all nodes to have an up-to-date copy of the entire input vector before an mxv operation, which is enforced via a sparsity- and mask-aware all-to-all communication. The communication cost for an mxv with dense vectors is proportional to the maximum amount of data any node sends or receives; i.e., $\Theta(n(p-1)/p) \approx \Theta(n)$. Since there is a constant number of mxv operations within HPCG and the number of benchmark iterations is controlled by the user, the total communication complexity of ALP is $\Theta(n)$. Similarly, synchronizations occur before every mxv operation, thus with a global synchronization cost of $\Theta(1)$.

The linear complexity of communication costs are expected to affect performance, as experiments in Section V confirm. Section VII further elaborates on this limitation, highlighting inherent limits of GraphBLAS and discussing mitigations.

We implement the RBGS smoother of Section III-A also in the reference HPCG code base available online [11]. From here on, we call this implementation *Ref.* Ref uses OpenMP to update the values within a single color in parallel in a shared memory system, together with MPI-3 primitives to exchange information among nodes for distributed execution; in particular, MPI Irecv/Isend are used to overlap execution and communication when updating the values of x for each color. Unlike Ref, the hybrid ALP/GraphBLAS backend uses blocking GraphBLAS semantics and thus features no such overlap. Like ALP (Section III-A), however, also Ref has $\Theta(n/p)$ work complexity.

The color-aware data exchange in Ref follows the same design principles in Section II-G, where each node exchanges with the geometrical neighbors only the values in its halo having the specific color to be updated. This keeps the same communication complexity derived in Section II-G: $\Theta\left(\sqrt[3]{n^2/p^2}\right)$. In Ref, neighboring nodes synchronize after updating each color. Since the number of colors found for

TABLE II: Details of the experimental machines; *italics* means per socket, otherwise per node.

	x86	ARM
СРИ	Xeon Gold 6238T	Kunpeng 920-4826
cores	22	48
threads	44 (HT enabled)	48
max frequency (GHz)	3.70	2.6
L3 cache (MB)	30.25	48
per core L2 cache (KB)	1024	512
memory channels	6	8
NUMA domains	1	2
sockets	2	2
RAM memory (GB)	192	512
max DDR frequency (MHz)	2933	2933
attained bandwidth (GB/s)	192	246.3
network adapter,		Mellanox ConnectX-5,
bandwidth		2x100Gb/s

HPCG does not depend on n or p, the total synchronization is again $\Theta(1)$. Table I summarizes the BSP asymptotic cost components of both ALP and Ref.

As in the original code base, Ref does not use any NUMAaware memory allocator, thus resorting to the standard domainlocal memory allocations of the C++ standard library implementation. The shared-memory and hybrid ALP/GraphBLAS backends, however, do perform NUMA-aware allocations.

V. EXPERIMENTAL RESULTS

This section discusses the experiments to validate the two implementations proposed in Section IV. Section V-A discusses the results on two systems: the first one is a dual-socket machine using an x86-64 architecture, here called *x86*; the second one is a dual-socket ARM64 machine, here called *ARM*. Table II shows the relevant hardware characteristics of both systems. Both employ Ubuntu Linux 20.04 and employ GCC 9 as compiler. Neither Ref nor ALP employ any architecturespecific library or instruction, thus remaining portable. An InfiniBand network interconnects up to 7 ARM machines, providing a cluster for scale-out experiments that Section V-B discusses; there, Ref uses the optimized OpenMPI distribution provided with the network adapter. Although multiple runs of the RBGS may improve convergence, HPCG performs by default one run, as this work does across all experiments.

All experiments achieve numerically comparable results, which allows fixing the number of iterations across all of them, thus making execution times directly comparable. Each experiment is repeated 10 times and the plots in this section show the average value. Unbiased standard deviations across experiments are negligible and thus not shown.

A. Results on shared memory

Figure 1 and Figure 2 show the strong scalability on both shared memory systems. In both plots, the x axis shows the number of application threads, increasing from less than those on a single socket to all those available on both sockets. To avoid caching effects, the problem size is set to the maximum that fits in the system memory, which is higher for ARM:



Fig. 1: Execution time of ALP and Ref with increasing number of threads on ARM



Fig. 2: Execution time of ALP and Ref with increasing number of threads on x86

this motivates the different time ranges between the two plots. Threads are pinned on physical cores, packing them on one socket if possible, i.e., with at most 48 threads on ARM and 22 threads on x86. Figure 2 also shows results with 44 threads on one socket (value "44 - 1S" on the *x* axis) and with 88 threads on two sockets (value "88 - 2S" on the x-axis), thus with hyperthreads. For the Ref results on two sockets, we test in both systems the default allocation policy as well as the interleaved one, enforced via the numactl command. As the latter always outperforms the former, the plots report only the interleaved Ref execution– thus assuming that the exploration regarding NUMA allocation is a common step for HPC practitioners, especially when dealing with multi-socket configurations.

Both Figure 1 and Figure 2 show that ALP outperforms Ref with all threads configurations. When the threads fit in



Fig. 3: Execution time of ALP and Ref with increasing number ARM nodes

one socket, ALP shows on both systems to saturate more quickly than Ref; this is due to the optimization available in ALP, where the GraphBLAS semantics and the C++ template-based implementation allow propagating rich information across software layers and to the compiler. In Figure 1, the performance of Ref slightly degrades when the number of threads approaches the number of cores on single socket, which we attribute to the NUMA-unaware allocation policy and to the two NUMA domains per socket. In Figure 2 with 44 threads pinned on a single socket (value "44 - 1S"), the two implementations are close, showing that Ref saturates only with hyperthreading; this suggests that ALP is more optimized.

B. Results on the distributed system

Figure 3 shows the results from weak-scaling experiments on a test cluster of ARM systems. These results confirm the asymptotic analysis in Table I. The Ref implementation shows a good weak scalability behavior, with execution times differing by at most 5% among different number of nodes, while the input size n grows proportionally to p.

Instead, the execution time of ALP increases linearly with the number of nodes, conform to Table I.

C. Scalability of Refinement/Restriction and RBGS

Figures 4-7 show the percentage of time spent in the MG kernel, split between the refinement/restriction kernels (dark bars) the and RBGS kernel (bright bars). The plots show the results for both implementations and for several setups, both shared memory and distributed; for each amount of compute resources (threads/nodes), the plots show the breakdown for each of the 4 coarsening levels (finer to coarser from left to right, respectively). The percentages refer to the total execution time, and the runtime in a given level does not include coarser levels. In all plots, MG (thus including RBGS) emerges as the main kernel of the entire HPCG simulation, with the aggregated MG execution time spanning from 80% to 90%



Fig. 4: Percentage of execution time spent in refinement/restriction (dark) and in RBGS (bright) for shared memory ALP on ARM



Fig. 5: Percentage of execution time spent in refinement/restriction (dark) and in RBGS (bright) for shared memory Ref on ARM

of the total execution time, while CG occupies the remaining 10% to 20% of the execution time. In turn, the aggregated execution of the RBGS smoother across all coarsening levels accounts for always more than 50% of execution time.

Figures 4 and 5 show the results for shared memory on ARM. Both refinement/restriction and the RBGS kernels show good scalability with many threads, with their percentage of runtime barely varying with respect to the total execution. In particular, in ALP the percentage of the two kernels slightly decreases with the increasing number of cores, while in Ref it fluctuates more clearly, probably due to the NUMA-unaware allocation policy. The results for x86 are qualitatively very similar, and thus not shown.

Instead, Figures 6 and 7 show the results for the distributed-



Fig. 6: Percentage of execution time spent in refinement/restriction (dark) and in RBGS (bright) for distributed ALP



Fig. 7: Percentage of execution time spent in refinement/restriction (dark) and in RBGS (bright) for distributed Ref

memory setup, where Ref spends a smaller percentage of time than ALP in refinement/restriction but a slightly higher one in RBGS. We attribute this to the multiple synchronization steps the implementation of RBGS within Ref, where for each color each node synchronizes with its neighbors. Instead, refinement/restriction is more expensive in ALP because it is implemented via an $m \times v$, which requires synchronization (as from Table I), while Ref directly accesses the vector data (as from Section II-F). For both implementations the percentages of execution time of the kernels remain very close across different numbers of nodes.

This observation, together with the good weak-scaling of Ref in Figure 3, shows that the chosen design scales well. The worse scalability behavior of ALP of Figure 3, in opposition to the good results in Figure 6, instead are caused by an inability to pass domain-dependent information to GraphBLAS.

VI. RELATED WORK

In the literature, multiple efforts are devoted to the optimization of the HPCG benchmark for different architectures. Architectures based on commodity CPUs are still common targets for HPCG, and vendors often made large efforts to showcase the capabilities of their architectures and the optimization strategies suitable for this benchmark: this is the case, among others, for x86 [28] and for ARM [20]. Similarly, HPCG implementations for CPU-based distributed architectures receive particular attention [21, 29].

Another body of work optimizes the benchmark for programmable accelerators like Intel Xeon Phi [28] or NVIDIA accelerators [30] at cluster scale. Accelerated solutions can be effective to achieve high performance, but need thorough optimizations and may exacerbate load-balancing issues. Indeed, some work also employs hypergraph partitioning strategies [31] to load-balance among heterogeneous nodes.

All of these solutions face the challenge of parallelizing the GS smoother, and typically resort to various implementations of RBGS together with a coloring algorithm, as this work does. Nonetheless, they devote large efforts to perform dedicated optimizations in order to exploit the underlying hardware. For example, [29] stresses on the importance of kernels fusion to improve access locality and save on bandwidth, a typical bottleneck for HPCG nowadays. Although fusion is a common compiler technique to achieve this goal, it is hard to perform it in an automatic fashion on complex code bases, especially if written with general-purpose programming languages like those traditionally used in HPC. Here, exploiting domain-specific information like the algebraic properties of operations required by the GraphBLAS specification can expose to the framework and the compiler many optimization and parallelization opportunities. Indeed, recent work [32] already proposes an extension of the current ALP/GraphBLAS implementation that fuses kernels corresponding to different GraphBLAS operations, showing large benefits in terms of locality and thus performance.

VII. CONCLUSIONS AND FUTURE WORK

This work presents a design of the HPCG benchmark on top of GraphBLAS, discussing the main kernels and their re-design for an effective implementation on top of standard algebraic operations. The code is available open-source together with ALP/GraphBLAS¹. The implementation on shared memory systems outperforms the reference one, bringing further evidence that expressing algorithms in a high-level, algebraic formulation enables a large spectrum of opportunities for automatic optimizations. Therefore, domain experts may attain both performance and productivity gains by pursuing an algebraic formulation of their problems.

Instead, the distributed-memory implementation shows fundamental scalability limitations compared to the reference, which leverages domain-specific geometrical information. For future work, Section VII-A discusses possible enhancements

¹https://github.com/Algebraic-Programming/ALP

that would especially benefit shared memory systems, while Section VII-B discusses the limitations for the distributedmemory parallelisation of HPCG, potential mitigations, and changes those would imply for GraphBLAS.

A. Improvements for shared memory systems

Domain-specific information can be beneficial for performance also in the case of a shared memory system. For example, the restriction and refinement operations in GraphBLAS in Section III-B must be materialized into a dedicated matrix, with storage and bandwidth costs. Instead, a GraphBLAS framework may be extended to allow a more abstract description of a linear operation, which may enable many compiler optimization and trade bandwidth for computation. Such an abstraction is possible when an operation can be described with few parameters, which is the case for restriction/refinement if we take into account the geometrical structure of the HPCG input. Although such abstract representation may not be feasible in domains like Algebraic Multigrids (AMRs), several workloads that operate on regularly structured sparse matrices, whether geometric in nature or not, may benefit.

Orthogonally, existing abstractions already allow pipelined execution of GraphBLAS operations [32], with benefits for data locality and performance under investigation.

B. Future work for distributed systems

Distributed systems fundamentally challenge the Graph-BLAS specification, in particular the opaqueness of containers: when domain-specific, geometrical information is lost or hidden in the nonzero pattern of a matrix, standard matrix distribution strategies usually cannot achieve the same scalability as domain-specific solutions. We describe four classes of solutions, dubbed i to iv, ordered by how much expertise is required by the GraphBLAS user. Solution A may hence be appropriate for *hero programmers* [33], which includes expert HPC programmers who typically compose and maintain code like HPCG. On the other end of the spectrum, solution D would be preferred by *humble programmers* [33] as it allows them to focus on the purely algebraic specification of the code, and not on details that affect performance or scalability.

- i) A definitive solution is to pass such domain-specific information to a GraphBLAS container so to explicitly give the implementation a preferred data *partitioning*, from which GraphBLAS may automatically derive a parallel work schedule for level-2 and 3 BLAS operations, both sparse and dense. Such annotation, however, 1) requires strong programmer expertise not only on their domain but also on the mapping of domain knowledge to linear algebra concepts, while 2) a framework implementing such a solution breaks the current GraphBLAS prescription of opaque containers. We dub this solution A, and proceed to discuss alternatives that alleviate these disadvantages.
- ii) Limiting the amount of programming effort required, multiple distributed backends with different matrix partitioning strategies may be provided. For example, a 2D matrix distribution instead of ALP/GraphBLAS current

1D decreases the communication cost in Table I from n(p-1)/p to $n/p(\sqrt{p}-1)$, thus only partially alleviating the communication bottleneck visible in the weak scaling experiment of Section V-B. This only partially improves on the current state and still requires some expert knowledge to understand how efficiently the input domain maps on the backend partitioning strategy.

- iii) One can leverage existing distributed data structures to describe grids and implement a GraphBLAS wrapper for these objects, allowing their use with linear algebraic operations. However, this solution depends on external software components and thus looses the performance guarantees of GraphBLAS. Another option is to extend GraphBLAS with the notion of grids, and provide matrix views of such objects; however, this escapes the intended scope of the GraphBLAS specification.
- iv) Finally, black-box partitioning methods may be used to automatically infer a partitioning of GraphBLAS matrices, with little to no user intervention. This reconstructs the domain information from the input itself, although at potentially significant pre-processing cost incurred while creating a GraphBLAS matrix, or may, at the cost of generality, incur this cost at compile time [34].

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