Report from Dagstuhl Seminar 23331

Recent Trends in Graph Decomposition

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Abstract

This report documents the program and the outcomes of Dagstuhl Seminar 23331 "Recent Trends in Graph Decomposition", which took place from 13. August to 18. August, 2023. The seminar brought together 33 experts from academia and industry to discuss graph decomposition, a pivotal technique for handling massive graphs in applications such as social networks and scientific simulations. The seminar addressed the challenges posed by contemporary hardware designs, the potential of deep neural networks and reinforcement learning in developing heuristics, the unique optimization requirements of large sparse data, and the need for scalable algorithms suitable for emerging architectures. Through presentations, discussions, and collaborative sessions, the event fostered an exchange of innovative ideas, leading to the creation of community notes highlighting key open problems in the field.

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1 Executive Summary

George Karypis (University of Minnesota – Minneapolis, US)
Christian Schulz (Universität Heidelberg, DE)
Darren Strash (Hamilton College – Clinton, US)

Large networks are useful in a wide range of applications. Sometimes problem instances are composed of billions of entities. Decomposing and analyzing these structures helps us gain new insights about our surroundings. Even if the final application concerns a different problem (such as traversal, finding paths, trees, and flows), decomposing large graphs is often an important subproblem for complexity reduction or parallelization. With even larger instances in applications such as scientific simulation, social networks, or road networks, graph decomposition becomes even more important, multifaceted, and challenging. The seminar was an international forum to discuss recent trends as well as to set new goals and new directions in this research area. The goal of this Dagstuhl Seminar was to bring algorithmic researchers from different communities together who implement, optimize, and/or experiment with algorithms running on large data sets or use techniques from the area frequently, thereby stimulating an exchange of ideas and techniques. The seminar focus was on graph decomposition. We chose the main topics of our seminar to bring experts together from a wide range of areas to tackle some of the most pressing open problems in the area of graph decomposition:

Hardware Design for Dealing with Graphs. Modern processors are optimized for computations that are floating point intensive and have regular memory accesses. Computations performed by sparse graph algorithms do not benefit from such optimizations. To address this mismatch, new processor and system architectures are being developed.

Beyond Smart Heuristics. In heuristic approaches, improvements in solution quality are often the result of a significant research effort. In recent years, to reduce this effort, develop better heuristics, and ultimately find better solutions, researchers have started developing approaches that use deep neural networks and reinforcement learning in order to learn those heuristics in an end-to-end fashion.

Formulations. Applications that process large sparse data generally have a unique set of optimization requirements for achieving the best performance. Parallelizing such applications on different architectures and/or using different frameworks introduces new performance issues that pertain to these architectures and frameworks. While graphs offer a rich ground for modeling such problems with different requirements, traditional graph decomposition tools may fall short to target those specific issues.

Scalable Parallel Algorithms for Future Emerging Architectures. Scalable high quality graph partitioning (with quality comparable to sequential partitioners) remains an open problem. With the advent of exascale machines with millions of processors and possibly billions of threads, the situation is further aggravated. Moreover, traditional "flat" partitions of graphs for processing on such machines implies a huge number of blocks. Efficient implementation is also a big issue since complex memory hierarchies and heterogeneity (e.g., GPUs or FPGAs) make the implementation complicated.

Summary of Seminar

The seminar convened 33 distinguished participants from both academic and industrial sectors worldwide. The majority of attendees arrived on Sunday evening. In total, the seminar showcased 19 presentations. The proceedings began with a welcome and ice-breaker session, facilitating introductions among participants. There were two dedicated sessions to address open problems. Ample time was set aside for collaboration. Additionally, a social event in the form of a hike was organized for attendees. The majority of the presentations were concise, spanning approximately 30 minutes, while a select few were of longer duration. Active discussions were a hallmark of this seminar, both during and after presentations, with highlights captured below. Spontaneous working groups emerged during the event, and their details are documented in the subsequent sections. During the week, we collaborated on a joint document that captures a large variety of open problems in the field. These so-called community notes which will be released/published in a separate document. Throughout and following the sessions, participants engaged in lively conversations. These discussions enriched the entire event and set it apart from typical conference formats. Beyond the research-focused activities, numerous social events like board games, poker, music evenings, hiking, and ping pong added a fun dimension. This made the seminar an excellent networking venue, especially for the many attendees experiencing Schloss Dagstuhl for the first time.

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3 Overview of Talks

3.1 Scalable Graph Clustering at Google

Jakub Lacki (Google – New York, US)

Graph clustering has numerous applications in classification, near-duplicate detection, data partitioning, community detection and privacy. In this talk we present a graph clustering library which supports all of these use cases and powers over a hundred applications at Google. One of the main design goals of the library is high scalability. In the offline setting, the library can handle up to trillion-edge graphs by leveraging distributed processing, or up to 100 billion edges using single-machine parallelism. Moreover, the library contains online algorithms that can update clustering with sub-second latency upon vertex insertions.

Discussions. There was a long discussion about applying ideas of TeraHAC to solving maximum weighted matching. In particular, both algorithms in the exact version find edges xy which are the highest weight incident edges for both x and y. In the approximate version of TeraHAC we relax this and allow almost-highest weight incident edges. We discussed whether this can be used to speed up greedy maximum weight matching and it looks like the idea may apply. However, showing asymptotic improvement in the running time bound seems to be somewhat harder. Another question that came up was how do we evaluate a near-dup clustering? We often use human raters that produce verdicts of the form: items x and y should/should not be in the same cluster. Lastly, when deciding about the similarity of two clusters x and y do we only look at edges between them, or do we also look at edges that go from x to outside of y (and vice versa)? Only edges between the clusters are considered.

3.2 Local Objectives for Graph Clustering

Katrin Casel (HU Berlin, DE)

In many situations clustering tasks do not involve (just) a global optimization goal, but (additionally) request local properties for clusters. Such local objectives are often particularly challenging. This talk gives some examples of such objectives for graph clustering with a brief overview of what is known and what is (surprisingly) open. In particular, these examples are connectivity and fairness as local objectives that are added to a global objective, density as difficult-to-check local objective, and chromatic edges where locally only the most prominent color counts.

Discussions. The talk gave rise to some new open questions: What happens when the dense partition objective is combined with a lower bound on the cluster size? Is connected partition in planar graphs easier than in general graphs? Discussions afterwards revealed: MaxMin/MinMax Balanced Partition inherits several hardness results from the Equitable Partition problem. Further, MaxMin/MinMax Balanced Partition is closely related to the Neighborhood Partitioning problem. The implications of this relationship remain to be investigated. Future studies should investigate, in particular from a computational point of view, which notion of fairness is most reasonable for Correlation Clustering (vertex vs edge fairness).

3.3 Parallel Incremental Clustering Algorithms for Massive Dynamic Graphs

Johannes Langguth (Simula Research Laboratory – Oslo, NO)

We consider the problem of incremental graph clustering where the graph to be clustered is given as a sequence of disjoint subsets of the edge set. The problem appears when dealing with graphs that are created over time, such as online social networks where new users appear continuously, or protein interaction networks when new proteins are discovered. For very large graphs, it is computationally too expensive to repeatedly apply standard clustering algorithms. Instead, algorithms whose time complexity only depends on the size of the incoming subset of edges in every step are needed. At the same time, such algorithms should find clusterings whose quality is close to that produced by offline algorithms. We discuss the computational model and present an incremental clustering algorithm, along with its parallel implementation. The scalability results suggest that our method is well suited for clustering massive graphs with acceptable running times while retaining a large fraction of the clustering quality.

Discussions. The performance of the incremental clustering algorithm depends heavily on the structure of the parts. So far, test instances have only been created by assigning edges to parts uniformly at random. Michael Fellows pointed out that different probability distributions would likely match actual growth of online social networks. Tobias Heuer pointed out that NCLiC does not actually compute modularity gains and that modularity retention could probably be improved by modifying the algorithm, although this might come at the cost of increased runtime. Jakub Lacki suggested to extend the incremental clustering algorithm from modularity maximization to correlation clustering which is certainly possible since the link-counting approach should work with many different clustering objectives. Ruben Mayer investigated the possibility of using NCLiC for streaming edge partitioning. Further discussion also suggested a way to replace the current way of randomly skipping expensive updates with an exact method by finding a suitable data structure.

3.4 Parameterized Approximation Schemes for Clustering with General Norm Objectives

Roohani Sharma (MPI für Informatik – Saarbrücken, DE)

We consider the well-studied algorithmic regime of designing a $(1+\epsilon)$-approximation algorithm for a k-clustering problem that runs in time $f(k,\epsilon)\text{poly}(n)$. Our main contribution is a clean and simple EPAS that settles more than ten clustering problems (across multiple well-studied objectives as well as metric spaces) and unifies well-known EPASes. Our algorithm gives EPASes for a large variety of clustering objectives (for example, k-means, k-center, k-median, priority k-center, ℓ-centrum, ordered k-median, socially fair k-median aka robust k-median, or more generally monotone norm k-clustering) and metric spaces (for example, continuous high-dimensional Euclidean spaces, metrics of bounded doubling dimension, bounded treewidth

metrics, and planar metrics). Key to our approach is a new concept that we call bounded ϵ-scatter dimension–an intrinsic complexity measure of a metric space that is a relaxation of the standard notion of bounded doubling dimension.

Discussions. After the talk, with Darren and Katrin we briefly discussed about the implementability of the presented algorithm. We summarized that though the power of the result in theory is that it gives a generalized framework for dealing with various clustering objective functions simultaneously, in order to implement it faster we need to do the proposed steps (for example finding a new center of the partial cluster) with a metric-sensitive algorithm.

3.5 Leveraging Learning-to-prune and reinforcement learning for solving combinatorial optimisation problems

Deepak Ajwani (University College Dublin, IE)

In recent years, machine learning (ML) techniques are being increasingly used for solving combinatorial optimisation problems. This often requires a deep integration between techniques from optimisation literature, algorithm engineering and machine learning. For instance, while the optimisation and algorithmic literature guides the feature engineering in learning models, the learning models can guide crucial design steps in exact MILP solvers as well as heuristics. Specifically, I would like to talk about the research done in my group on a range of combinatorial optimisation problems in graphs such as variants of vehicle routing problems, Max Cut, Max Clique, Steiner tree etc. We have used a combination of supervised techniques such as learning-to-prune, reinforcement learning techniques such as CombOptZero and some recent unsupervised learning techniques to compute high quality solutions to optimisation problems in an efficient and scalable manner. In addition, we have also explored if learning techniques can speed up local search heuristics.

Discussions. There seemed to be a general agreement about my main argument that in order for a learning technique to (i) have a simple, interpretable architecture, (ii) generalise to larger sizes and (iii) work effectively with limited training data, it will likely have to be integrated with techniques from optimisation and algorithm engineering communities. The questions were mostly geared towards better understanding of the learning models and the associated details, such as how to label the data in case of multiple optimal solutions and what to do with integer linear programs that are non-binary etc. There were some discussions on how to apply these techniques to reduce the problem size and improve the refinement part (some of this is also noted in the open problem section). There were also discussions on how effectively reduction rules and kernelization techniques can be leveraged in the learning frameworks that I presented. Also, I was pointed to interesting references in this area such as Frederic Manne's work on using GNN for learning vertex cover [1], the linked paper on heuristics for hitting set[2] and on "Graph Partitioning and Sparse Matrix Ordering using Reinforcement Learning and Graph Neural Networks"[3].

[1] https://drops.dagstuhl.de/opus/volltexte/2022/16546/
[2] https://epubs.siam.org/doi/pdf/10.1137/1.9781611977042.17
[3] https://arxiv.org/abs/2104.03546

3.6 Using Steiner Trees in Hypergraph Partitioning

Tobias Heuer (Karlsruhe Institute of Technology, DE)

Minimizing wire-lengths is one of the most important objectives in the realization of modern circuits. The design process involves initially placing the logical units (cells) of a circuit onto a physical layout, and subsequently routing the wires to connect the cells. Hypergraph partitioning (HGP) has been long used as a placement strategy in this process. However, it has been replaced by other methods due to limitations of existing objective functions for HGP, which only minimizes wire-lengths implicitly. In this talk, we present a novel HGP formulation that maps a hypergraph H, representing a logical circuit, onto a routing layout represented by a weighted graph G. The objective is to minimize the total length of all wires induced by the hyperedges of H on G. To capture wire-lengths, we compute minimal Steiner trees – a metric commonly used in routing algorithms. For this formulation, we present a direct k-way multilevel algorithm that we integrate into the shared-memory hypergraph partitioner Mt-KaHyPar. Mt-KaHyPar is a highly scalable partitioning algorithm that achieves the same solution quality as the best sequential algorithms, while being an order of magnitude faster with only ten threads. Our experiments demonstrate that our new algorithm achieves an improvement in the Steiner tree metric by 7% (median) on VLSI instances when compared to the best performing partitioning algorithm that optimizes the mapping in a postprocessing step. Although computing Steiner trees is an NP-hard problem, we achieve this improvement with only a 2–3 times slowdown in partitioning time compared to optimizing the connectivity metric.

Discussions. In the talk, Tobias used wire-length minimization as the main objective for VLSI design and motivation for my novel hypergraph partitioning formulation. However, attendees rightly noted that this is just one of several important metrics, such as, e.g., the perimeter of bounding boxes around nets. Additionally, some mentioned that placement challenges have been addressed using reinforcement learning recently.

3.7 Directed Acyclic Partitioning from Graphs to Hypergraphs

Ümit V. Çatalyürek (Georgia Institute of Technology – Atlanta, US)

Data transfer continues to be the biggest obstacle to efficient computation. The de facto abstraction for modeling computations has been directed acyclic graphs (DAGs). When scheduling computational tasks, an effective load balance and data locality trade-off is required. The ordering and mapping of the DAG's vertices (i.e., tasks) to computational resources are significantly benefited by acyclicity. As a result, it is preferable to maintain acyclicity at various levels of computation. In this talk, we demonstrate how acyclic partitioning of DAGs – partitioning where the inter-part edges of vertices from different parts should preserve an acyclic dependency among the parts – can be investigated to reduce redundant data movement on two-level memory settings. We also present the challenges of developing acyclic partitioning methods for directed hypergraphs, where they provide more elegant and accurate abstractions than graph counterparts.

Discussions. George Karypis was suggesting a potential alternative model for DAG partitioning for quantum simulation, with one fixed partition, to model the problem as edge-cut partitioning. In offline discussions, it turned out that the model doesn't fit the problem that is solved here.

3.8 Approximate Modular Decomposition

Yosuke Mizutani (University of Utah, US)

One fruitful avenue for designing efficient graph algorithms has been to parameterize using a variety of structural parameters (e.g. treewidth, clique-width) in addition to the natural parameter (i.e. solution size). Modular-width is a structural parameter introduced by Gajarsky et al. (2013) in an effort to generalize simpler notions on dense graphs while avoiding the intractability that often came with the existing clique-width parameter. Modular-width has several additional advantages – it can be computed in linear-time, and the associated modular decomposition (MD) tree has applications in visualization and parallel processing. Unfortunately, real-world graphs tend to have large modular-width. This leads us to the following natural questions: given a graph G, is there a useful notion of approximate MD trees that preserves fast computation, exhibits much lower widths, and enables solution of the downstream problems with quality guarantees? There are several possible avenues of attack. For example, we could define a graph editing problem: can we make a small number of changes to G to produce a G' with low modular-width? Another formulation would be to relax the definition of modules, which is likely closely interwoven with the idea of twin-width. Finally, we consider the option of taking a data-driven approach. What kind of graphs admit a nice approximation of modular decomposition?

3.9 Exact k-way sparse matrix partitioning

Rob H. Bisseling (Utrecht University, NL)

Joint work of Engelina Jenneskens

To minimize the communication in parallel sparse matrix-vector multiplication while maintaining load balance, we need to partition the sparse matrix optimally into k disjoint parts, which is an NP-complete problem. We present an exact algorithm and an implementation called General Matrix Partitioner (GMP) based on the branch and bound (BB) method which partitions a matrix for any k, and we explore exact sparse matrix partitioning beyond bipartitioning. We also present an integer linear programming (ILP) model for the same problem, based on a hypergraph formulation. We used both methods to determine optimal 2,3,4-way partitionings for a subset of small matrices from the SuiteSparse Matrix Collection. To answer the question "How good is recursive bipartioning (RB)?", we used the exact results found for $k = 4$ to analyse the performance of RB with exact bipartitioning. Finally, we will discuss how exact methods inspire heuristic methods such as medium-grain partitioning and we will briefly touch on heuristic solvers such as Mondriaan and its hybrid distributed/shared-memory parallel version PMondriaan, which is currently under development.

Discussions. George Karypis asked whether there are worst-case results about the quality of recursive bipartitioning. There are papers like by Shang-Hua Teng and Horst Simon about possibly bad partitionings by RB, but the results of the talk show that they do not occur in practice for the small problems tested. Sherry Li asked about the realism of communication volume as a metric reflecting communication time. It is true that you want to minimise total communication volume as wel as per processor volume, and also the latency. Since data words communicated to the same processors can be combined into one message, the latency can be significantly reduced, and will only be a problem for a very large numbers of processors and a relatively small problem size. Tobias Heuer asked what splitting hyperedges exacly means. This feature is incorporated in the version of PMondriaan to be released, and it can be exemplified by converting hyperedges of size 3 into 3 edges of size 2, and then combining them with other edges and correcting where needed for the cost.

3.10 What Scotch cannot do yet

François Pellegrini (University of Bordeaux, FR)

In 30 years, the Scotch software has seen many increases in its capabilities. However, like its (friendly) competitors, its functional envelope is limited. In this talk, we will discuss problems that Scotch is not yet able to solve, and how to address them in the (near) future.

Discussions. By the end of the presentation, two open problems were presented. The first one relates to approximating distances in a family of recursively coarsened graphs, with respect to the distance computed in an initial fine graph. The aim of this method would be to avoid handling $O(p^2)$ distance matrices for all target graph vertices (where p is the number of such vertices). During the discussion, it was mentioned that software for car traffic routing also use multilevel descriptions of the distances between locations [Sebastian], and that partial matrices are built, or local distance computations, are performed for each level. The case for tree-shaped architectures was also discussed [Henning], but answers are straightforward with this architecture. The second open problem relates to the computation of distance-2 coloring of a graph, which is a prerequisite to run a subsequent deterministic, lock-free matching algorithm. The discussion [Bora, Fredrik] converged to the fact that if the final goal of obtaining a deterministic matching was sought, directly using a locking algorithm could do faster for a small number of threads.

3.11 Recent Advances in Streaming (Hyper)Graph Decomposition

Marcelo Fonseca Faraj (Universität Heidelberg, DE)

There is a gap in (hyper)graph decomposition algorithms. Streaming algorithms, which are adaptable to small machines, partition huge (hyper)graphs quickly, but yield low-quality results. Conversely, in-memory algorithms produce high-quality solutions but require significant memory. Our talk explores recent advances in streaming (hyper)graph decomposition. We

begin with streaming graph partitioning, covering from hash-based to buffered approaches. Next, we discuss the state of the art in streaming process mapping. Finally, we present recent advances in streaming hypergraph partitioning. With their recent introduction and potential for further improvement, these families of streaming algorithms present unexplored avenues for improvement, while their recent strong results can provide new insights into solving the respective in-memory versions of these problems.

Discussions. There were some discussions if the degree of a vertex is currently considered in the local opbjective function that is optimized by the streaming graph partitioning algorithm. Currently this is not the case, but this may be interesting to consider in the future. Moreover, Tobias Heuer mentioned that the buffered streaming model for streaming graph partitioning could also be extended to hypergraph partitioning yielding potentially higher solution quality for hypergraph streaming partitioners.

3.12 Graph partitioning and distributed graph processing – An end-to-end optimization perspective

Ruben Mayer (Universität Bayreuth, DE)

Graph partitioning is often considered as a necessary preprocessing step for distributed graph processing. In doing so, the partitioning quality in terms of cut size and balancing is crucial to the performance of distributed graph processing jobs. However, yielding high graph partitioning quality is a challenging and compute-intensive problem. Many different graph partitioning algorithms have been proposed, which differ both in their achieved partitioning quality as well as their computational costs. How many resources and how much time to invest into partitioning depends on various factors such as the graph size, the resource budget of the user, and the complexity and run-time of subsequent graph processing on the partitioned graph. In my talk, I will elaborate on the problem of optimizing the end-to-end graph processing pipeline.

Discussions. There were several questions during the talk. For example, what can we learn from the trained ML models in EASE about the workloads under which certain partitioners perform best and how much of the graph in HEP is high-degree vs. low-degree, especially whether there are significant high-degree parts.

3.13 Parameterized complexity and algorithmics – some horizons – and the universal applied paradigm of diverse solutions

Mike Fellows (University of Bergen, NO)

The talk will describe in a very accessible way the foundational motivations and brief formal setup of parameterized complexity, a name which has too many syllables, but it is pretty straightforward and can be compared to “coordinatized geometry”. It has always

been nurtured as a theory, with the aspiration to be useful in practice. It goes beyond the one-dimensional P versus NP framework in a quite simple way, much as coordinatized geometry went beyond the Geometry of the Greeks. One natural way to usefully deploy parameterization is to address the working reality of many computing applications domains: that a single mathematically optimal solution is not what is really wanted! In many practical computing applications areas, what is really wanted is a moderate-sized collection of quality-wise pretty good solutions to choose from, often on the basis of side information not included in the strict optimal mathematical model. The talk is based on a recent IJCAI paper with multiple authors that began this direction of research, that fits very neatly with the mathematical algorithm design tools of parameterized complexity.

3.14 Combinatorial problems in sparse matrix computations

Xiaoye S. Li (Lawrence Berkeley National Laboratory, US)

We will describe the combinatorial algorithms needed in sparse matrix computations for solving algebraic equations. We will focus on the open problems in the graph preprocessing stages, such as ordering, symbolic factorization, and communication schedule, and particularly the speculations on the multi-GPU design.

Discussions. George Karypis mentioned that there isn't any refinement used specifically for the vertex separator. There was some discussion that involved multiple iterations of Luby's algorithm to increase the size of the computed independent set (and hence decrease the size of the computed vertex cover). Sherry clarified that, at present, they only use a single iteration, although he acknowledged that there's potential to enhance its quality. The two delved deeper into the concept of multilevel refinement. In this context, there were dicussions if and how combinations of mindegree and nested dissections, which have proven to be effective in practice, had been considered.

3.15 Algebraic Programming for Graph Computing: GraphBLAS and beyond

Albert-Jan Yzelman (Huawei Technologies – Zürich, CH)

Evolving from GraphBLAS, Algebraic Programming, or ALP for short, requires programmers to annotate their programs with explicit algebraic information. This information is then used in auto-parallelisation and other automatically applied optimisations, ranging from low-level concerns such as vectorisation to more complex algorithmic transformations. Recent work revolves around achieving faster parallel performance chiefly via non-blocking execution, providing more humble programming interfaces beyond GraphBLAS' generalised sparse linear algebra, and introducing a system for structured data representation. This talk will briefly introduce the status of ALP as-is, the guiding ideas behind its design, and a summary of recent advances. It then focuses on challenges towards increasing the usability and applicability

of ALP, as well as on challenges in bridging the state of the art in combinatorial scientific computing algorithms –such as partitioners or schedulers– for improving the performance of ALP-based programs.

Discussions. There was a discussion regarding the scope of algebraic programming, in particular if it is exclusively tied to GraphBLAS, Albert-Jan Yzelman clarified that algebraic programming is not restricted to just GraphBLAS. In fact, the domain encompasses a wide variety of applications and tools.

3.16 Distributed Landmark Labelling Using Vertex Separators

Kamer Kaya (Sabanci University – Istanbul, TR)

Distance queries are a fundamental part of many network analysis applications. Distances can be used to infer the closeness of two users in social networks, the relation between two websites in a web graph, or the importance of the interaction between two proteins or molecules. As a result, being able to answer these queries rapidly has many benefits to the area of network analysis as a whole. Pruned landmark labeling (PLL) is a technique used to generate an index for a given graph that allows the shortest path queries to be completed in a fraction of the time when compared to a standard breadth-first or a depth-first search-based algorithm. Parallel Shortest-distance Labeling PSL reorganizes the steps of PLL for the multithreaded setting and works particularly well on social networks. Unfortunately, even for a medium-size, 50 million vertex graph, the index size can be as large as 300GB. On the same graph, a single CPU core takes more than 12 days to generate the index. This presentation is on a distributed algorithm by partitioning the input graph. The proposed method improves both the execution time and the memory consumption by distributing both the data and the work across multiple nodes of a cluster.

Discussions. There was some discussion on how the graph can be better partitioned and how the algorithm can be modified for vertex/edge additions/deletions. The size of the index for larger graphs was questioned and the best possible performance we can was also discussed briefly.

3.17 Recent Advances in Ka (Hyper)Graph Partitioning

Daniel Seemaier and Lars Gottesbüren (KIT – Karlsruher Institut für Technologie, DE)

In the first part of our talk, we will present a brief overview of our two main solvers Mt-KaHyPar and KaMinPar for balanced (hyper)graph partitioning. Until recently, there was a severe gap in terms of solution quality between sequential and parallel solvers. We have since parallelized all of the techniques in sequential solvers that lead to high solution quality, which are now available in Mt-KaHyPar. Moreover, we tackled new problem domains such as efficiently partitioning into a very large number of clusters with the deep multilevel scheme,

which is available in KaMinPar. Additionally, KaMinPar was recently extended with a high-performance MPI mode, adapting the deep multilevel scheme to the distributed scenario. In the second part of our talk, we will then present some currently ongoing work. Traditionally, local search algorithms perform only balance-preserving moves. Perhaps unsurprisingly, we can achieve huge quality improvements by permitting large balance violations; performing unconstrained moves with some caution and rebalancing the solution later on. The same quality gap that used to exist between sequential and shared-memory parallel, now exists between shared-memory parallel and distributed-memory partitioners. Therefore, we are working on a distributed FM version in KaMinPar, as well as a distributed version of the recently proposed JET algorithm, both of which show promising results in preliminary experiments.

Discussions. The discussions revolved around the topics of scalability and problem formulations. Specifically, how many cores are needed for Mt-KaHyPar to be faster than PaToH (2 cores), why does the deterministic version scale better than the non-deterministic versions (because non-determinism may incur additional rounds needed to converge) and matters of parallel programming.

3.18 Graph Neural Network Research at AWS AI

George Karypis (University of Minnesota – Minneapolis, US)

During just a few years, Graph Neural Networks (GNNs) have emerged as the prominent supervised learning approach that brings the power of deep representation learning to graph and relational data. An ever-growing body of research has shown that GNNs achieve state-of-the-art performance for problems such as link prediction, fraud detection, target-ligand binding activity prediction, knowledge-graph completion, and product recommendations. As a result, GNNs are quickly moving from the realm of academic research involving small graphs to powering commercial applications and very large graphs. This talk will provide an overview of some of the research that AWS AI has been doing to facilitate this transition, which includes developing the Deep Graph Library (DGL)–an open source framework for writing and training GNN-based models, improving the computational efficiency and scaling of GNN model training for extremely large graphs, developing novel GNN-based solutions for different applications, and making it easy for developers to train and use GNN models by integrating graph-based ML techniques in graph databases.

3.19 An MPI-based Algorithm for Mapping Complex Networks onto Hierarchical Architectures

Henning Meyerhenke (HU Berlin, DE)

Processing massive application graphs on distributed memory systems requires to map the graphs onto the system's processing elements (PEs). This task becomes all the more important when PEs have non-uniform communication costs or the input is highly irregular.

Typically, mapping is addressed using partitioning, in a two-step approach or an integrated one. Parallel partitioning tools do exist; yet, corresponding mapping algorithms or their public implementations all have major sequential parts or other severe scaling limitations. In this paper, we propose a parallel algorithm that maps graphs onto the PEs of a hierarchical system. Our solution integrates partitioning and mapping; it models the system hierarchy in a concise way as an implicit labeled tree. The vertices of the application graph are labeled as well, and these vertex labels induce the mapping. The mapping optimization follows the basic idea of parallel label propagation, but we tailor the gain computations of label changes to quickly account for the induced communication costs. Our MPI-based code is the first public implementation of a parallel graph mapping algorithm; to this end, we extend the partitioning library ParHIP. To evaluate our algorithm's implementation, we perform comparative experiments with complex networks in the million- and billion-scale range. In general our mapping tool shows good scalability on up to a few thousand PEs. Compared to other MPI-based competitors, our algorithm achieves the best speed to quality trade-off and our quality results are even better than non-parallel mapping tools.

Discussions. The discussion after the talk revolved around various aspects: (i) the advantages and disadvantages of modeling the system architecture by a tree, (ii) implementation aspects regarding high-degree vertices, and (iii) the straightforward extension to reordering with the proposed approach. Furthermore, some pointers to additional related work were provided.

4 Working Groups

4.1 Balanced Edge Partitioning for Distributed Graph Processing

Ruben Mayer (Universität Bayreuth, DE)

The generally accepted formulation of the edge partitioning problem imposes a load balancing constraint on the number of *edges* per partition: $\forall p_i \in P : |p_i| \leq \alpha * \frac{|E|}{k}$ for a given $\alpha \geq 1, \alpha \in \mathcal{R}$, where $|p_i|$ denotes the number of edges in partition p_i. However, balancing only the number of edges does not always lead to good load balancing in distributed graph processing. In some cases, it is better to balance the number of vertex replicas. The open problem is to achieve an edge partitioning that is balanced both in the number of edges and vertices while minimizing the vertex replication factor. First thoughts in that direction may lead to the formulation of a multi-constraint partitioning problem. The working group discussed various models that could be used to achieve that, i.e. modelling the problem as a multi-constraint hypergraph or matrix partitioning problem.

4.2 Edge-Colored Clustering

Blair D. Sullivan (University of Utah – Salt Lake City, US)

This working group discussed the Edge-Colored Clustering problems presented in Thursday morning's Open Problem session, which relate to issues in clustering hypergraphs with categorical edge labels. The group began by trying to relate the non-overlapping variant of the problem to hypergraph partitioning without balance constraints. They also considered whether the locally budgeted overlap problem is equivalent to a generalization of vertex cover (in particular, b-coloring was discussed), eventually resulting in a family of graphs for which the two problems diverge arbitrarily. In addition to trying to relate ECC to previously-studied problems, the group also discussed (in)approximability, data reduction/kernelization, the possibility of using ILP solvers, and practical use-cases.

4.3 Exact k-way sparse matrix partitioning

Rob H. Bisseling (Utrecht University, NL)

Robust ILP methods have consistently demonstrated superior performance over Brand and Bound when it comes to matrix partitioning. Delving deeper into the intricacies of these solvers reveals a myriad of complex processes at work. The question arises: what unique advantages do ILPs offer in the realm of sparse matrix and graph partitioning? What insights can we glean from their application and functionality? This was discussed in part in the working group. Interestingly, when ILP is applied during the initial partitioning phase, it often paves the way for potential improvements. However, it's worth noting that these enhancements, while promising, can come at a significant cost. And surprisingly, in the context of initial partitioning, they might not always translate into better overall results. Could there be something valuable to extract from the pre-solve and branch-and-bound techniques employed in these solvers? Such insights could be revolutionary, especially given the current limitations of solvers when dealing with dense networks. Furthermore, there was an emerging discourse surrounding parallel solvers. It's essential to emphasize this area as it holds significant promise and potential for future developments in matrix partitioning techniques.

5 Open Problems

In the last four decades, there has been a tremendous amount of research in the area of the seminar. See for example the book by Bichot and Siarry [7], the survey by Schloegel et al. [67] or Kim et al. [32] as well as last generic surveys on the topic by Buluç et al. [10] and more recently Çatalyürek et al. [14]. However, a wide range of challenges remain in the area. Thus we now report currently open problems and future directions in the area of (hyper)graph decomposition that have been presented during Dagstuhl Seminar 23331 on "Recent Trends in Graph Decomposition".

5.1 Preliminaries

A *weighted undirected hypergraph* $H = (V, E, c, \omega)$ is defined as a set of n vertices V and a set of m hyperedges/nets E with vertex weights $c : V \to \mathbb{R}_{>0}$ and net weights $\omega : E \to \mathbb{R}_{>0}$, where each net e is a subset of the vertex set V (i.e., $e \subseteq V$). The vertices of a net are called *pins*. We extend c and ω to sets in the natural way, i.e., $c(U) := \sum_{v \in U} c(v)$ and $\omega(F) := \sum_{e \in F} \omega(e)$. A vertex v is *incident* to a net e if $v \in e$. $\mathrm{I}(v)$ denotes the set of all incident nets of v. The set $\Gamma(v) := \{u \mid \exists e \in E : \{v, u\} \subseteq e\}$ denotes the neighbors of v. The *degree* of a vertex v is $d(v) := |\mathrm{I}(v)|$. We assume hyperedges to be sets rather than multisets, i.e., a vertex can only be contained in a hyperedge *once*. Nets of size one are called *single-vertex* nets. Given a subset $V' \subset V$, the *subhypergraph* $H_{V'}$ is defined as $H_{V'} := (V', \{e \cap V' \mid e \in E : e \cap V' \neq \emptyset\})$.

A *weighted undirected graph* $G = (V, E, c, \omega)$ is defined as a set of n vertices V and a set of m and edges E with vertex weights $c : V \to \mathbb{R}_{>0}$ and edge weights $\omega : E \to \mathbb{R}_{>0}$. In contrast to hypergraphs, the size of the edges is restricted to two. Let $G = (V, E, c, \omega)$ be a weighted (directed) graph. We use *hyperedges/nets* when referring to hypergraphs and *edges* when referring to graphs. However, we use the same notation to refer to vertex weights c, edge weights ω, vertex degrees $d(v)$, and the set of neighbors Γ. In an undirected graph, an edge $(u, v) \in E$ implies an edge $(v, u) \in E$ and $\omega(u, v) = \omega(v, u)$.

5.2 Balanced (Hyper)graph Decomposition and Variations

Balanced Hypergraph Partitioning

Multilevel Scheme. Although traditional coarsening algorithms work particularly well for mesh graphs, their extension to hypergraphs has revealed a lack of understanding and can easily destroy the structure of the hypergraph. It is important to invest in better coarsening techniques tailored specifically to hypergraphs to preserve their structural properties. An interesting avenue in that direction could be incorporating embeddings during coarsening. By leveraging embeddings, coarsening algorithms could potentially achieve better representations of hypergraph structures, leading to improved partitioning outcomes. While spectral techniques were popular in the pre-multilevel era, pure spectral partitioning was not deemed competitive afterwards – mainly due to high running times. With the increased performance of today's machines and GPUs, it might be worthwhile to revisit these approaches as multilevel refinement techniques. Recently, unconstrained refinement (ignoring balance constraint while performing node moves) with subsequent rebalancing has shown promising results. However, the design space of these types of algorithms is far from being explored.

Methodology. Currently, we are lacking evaluations of real-world applications and workflows that use partitioning for load balancing and communication volume minimization. Therefore, the impact of quality gains in partitioning in terms of running time improvements for the applications are somewhat unclear. Moreover, in both graph and hypergraph partitioning, we still don't have a uniformly accepted balance constraint definition that works well in the case of vertex weighted (hyper)graphs. There exist definitions that enforce a lower bound on the block weights, add the weight of the heaviest vertex to the balance definition, or simply require that each block must be non-empty. Given that finding a balanced partition is an NP-hard problem even without optimizing an objective function, we should investigate in a balance definition that guarantees the existence of a feasible solution without providing too much leeway in the maximum allowed block weights.

High-Quality Distributed-Memory Partitioning. In recent years, several publications demonstrated that shared-memory partitioning algorithms can achieve the same solution quality as their sequential counterparts. However, the same quality gap still exists between sequential and distributed-memory solvers.

Bottleneck Objective Functions. For parallel computations, we assign the nodes of a (hyper)graph evenly to processors in a computing cluster. This should balance the computational load across the cluster. However, this does not bound the communication between processors, which can also become a sequential bottleneck if some PEs have to communicate significantly more than others. Therefore, we should investigate in techniques for optimizing bottleneck objective functions.

The One Partitioning Tool Idea. The graph- and hypergraph partitioning problems come in many different flavors: weighted vs. unweighted (hyper)graphs, directed vs. undirected hypergraphs, different objective functions, single vs. multi-objective, single vs. multi-constraint, partitioning with fixed vertices, partitioning with variable block weights, etc. Can we join forces and build (upon) a single open-source multilevel framework that is easily extensible to foster the research and development of new partitioning heuristics such that we can have a single tool that actually is able to solve all of these problems?

(Hyper)DAG Scheduling

Let a HyperDAG (or, alternatively, a DAH – directed acyclic hypergraph) represent a computation and be given by a set of vertices and directed hyperedges, i.e., $\mathcal{H} = (\mathcal{V}, \mathcal{N})$. Here, $\mathcal{V} = \mathcal{S} \cup \mathcal{T} \cup \mathcal{O}$ while every directed hyperedge $n \in \mathcal{N}$ consists of a source and an arbitrary number of destination vertices; i.e., $n \in \mathcal{V} \times \mathcal{P}(\mathcal{V})$, where $\mathcal{P}(\mathcal{V})$ is the power set of $\mathcal{V}$. The vertices $\mathcal{S}$ are the input (source) data of the computation, the outputs are in $\mathcal{O}$, while intermediate computations are captured by computing *tasks* in $\mathcal{T}$.

Scheduling the computation on a parallel system with p processing units requires assigning each vertex $v \in V$ a time step t_v and a location $s_v \in \{0, 1, \ldots, p-1\}$ that define when and where to execute the intermediate computation in the case of $v \in \mathcal{T}$, or when and where an input (or output) should be available in the case of $v \in \mathcal{S}$ (or $v \in \mathcal{O}$).

Let us initially consider a machine model that costs communication and computation, though does not consider weights for simplicity of presentation – i.e., each data element $v \in \mathcal{S} \cup \mathcal{O}$ uniformly costs some unit storage; $v \in \mathcal{T}$ generates intermediate data that costs the same unit storage; and $v \in \mathcal{T}$ costs some unit time to compute.

Approaching the scheduling problem from a hypergraph partitioning point of view generates a mutually disjoint $\mathcal{V}_0, \ldots, \mathcal{V}_{p-1}$ partition of $\mathcal{V}$ under some allowed load imbalance ϵ, and minimizes the traditional $\lambda-1$-metric $\sum_{n_i \in \mathcal{N}} (\lambda_i - 1)$; i.e., minimizes the communication volume of data units between parts of the partition[4]. However, even a perfectly balanced and optimal partitioning may lead to a division of the HyperDAG across the p compute units that exposes no parallelism whatsoever. One solution is to divide the HyperDAG into s layers $\mathcal{L}_0, \ldots, \mathcal{L}_{s-1}$, where vertices $v \in \mathcal{L}_{\leq i}$ are predecessors of those in $\mathcal{L}_{>i}$, and then to partition each layer separately. Recent results show, amongst other results, that the resulting HyperDAG partitioning problem is NP-hard, and also that no polynomial-time approximation algorithm exists [52]. An additional problem is determining an appropriate s, which is a hard problem on its own.

[4] Here, λ_i is defined as the *connectivity* of the ith hyperedge, i.e., the number of parts of the partition the vertices in that hyperedge span.

Optimal Scheduling. Similar in motivation to the sparse matrix partitioning problem in Section 5.2 in this paper, one challenge is to find optimal schedules for real-world HyperDAGs. A collection of problems may be found in open HyperDAG_DB repository[5], which welcomes additional problem submissions. Determining optimal schedules enables efficient execution of oft-repeated computations, such as those in training neural networks; enables gauging the effectiveness of current heuristics for online scheduling, such as those used within run-time systems like OpenMP or Cilk; and enables inspiring better on-line heuristics by looking at optimal examples. This direction implies finding better ILP formulations and improved pruning strategies for use with optimal scheduling algorithms. Pruning strategies may furthermore rely on data-driven methods, see e.g., Juho et al. [39], trained using entries of the HyperDAG database that have been solved to optimality.

Models and Hardness. The hardness results previously presented depend on assumptions on the underlying machine and cost models. Indeed, other choices may reveal differing hardness results– for example, the same recent work shows that removing the layer-wise constraint in favor of a makespan constraint on the HyperDAG partitioning results in an optimization problem where *evaluating* whether said constraint has been violated is an NP-hard problem in itself [52]. A fundamental challenge thus is to identify what machine and cost model choices

1. result in significantly harder optimization problems,
2. affect the search space underlying the optimization problem and how, and
3. have optimal schedules that relate to one another and how.

Example modeling choices include whether time step assignment takes place at the unit vertex granularity or in bulk (e.g., assigning multiple tasks to a single layer); whether data between vertices are moved individually or in bulk; whether communication in a time step charges constant latency, a cost proportional to a size, or both; whether communication size corresponds to volume or h-relations[6]; whether communication may overlap with computation; or whether communication throughput and latency (when costed) are uniform across the p processing units, or instead hierarchical or even topology-dependent. More detailed initial considerations on such modeling options appear in a pre-print [51].

To make each of the three above challenges more concrete, we briefly follow with known examples: 1+2) electing a machine model where vertex-to-time-step assignment happens in bulk and layer-wise, leads to fewer variables in an ILP formulation and thus to a reduced search space; yet, paradoxically, also has stronger known hardness results compared to non-layered hypergraph partitioning [52]; 3) there is at most a factor two difference between optimal BSP solutions[7] with overlapping communications versus those without.

(Hyper)graph Algorithms and ALP

Algebraic programming, or ALP for short, enables writing programs with explicit algebraic information passed into the programming framework. Examples of such algebraic information are binary operators and their properties such as associativity, commutativity, etc., as well as richer algebraic structures such as monoids and semirings. A semiring embodies the

[5] `https://github.com/Algebraic-Programming/HyperDAG_DB/`

[6] the maximum of incoming and outgoing messages to or from any partition at a given time step.

[7] with BSP, compute tasks and communication are considered in bulk, communication charges both latency and size, communication size is given by h-relations, and latency as well as throughput parameters are uniform [78].

rules under which linear algebra takes place, but allows its generalization to any pair of additive and multiplicative operations under which those rules hold; for example, while the plus-times semiring enables standard numerical linear algebra, the min-plus semiring enables shortest-paths computations. The following two observations are core to GraphBLAS: a) most graph algorithms can be expressed in (generalized) linear algebra; and b) our deep understanding of optimizing sparse linear algebra (thus) applies to graph computations.

The recent nonblocking mode of ALP/GraphBLAS performs fusion of linear algebraic primitives under any algebraic structure, at run-time. It achieves up to 16.1× and 12.2× speedup over the similar state-of-the-art frameworks of SuiteSparse:GraphBLAS and Eigen on ten matrices for the PageRank algorithm, with similar results for a Conjugate Gradient (CG) solver and sparse deep neural network inference [46, 45]. Other recent work introduces support for dense linear algebra, matrix structures (e.g., triangular), and views (e.g., permutations or outer products) [71]. It furthermore enables automatic distributed-memory execution of sequential ALP code [86, 68].

ALP Accelerating Graph Algorithms. With the new extensions, both the applicability and performance of the ALP framework has increased, and should enable the acceleration of graph algorithms that previously only had sequential or otherwise un-optimized representations. To aid porting efforts, ALP not only supports the auto-parallelization of linear algebraic formulations of graph problems, but also that of vertex-centric ones [82].

One challenge is to find graph algorithms that, despite recent advances, remain hard to express using generalized linear algebra, or graph algorithms that are expressible yet do not achieve high performance. Examples include k-core decomposition and p-spectral clustering, the former done successfully [41] and the latter still partially relying on non-ALP code [53].

Graph Algorithms Accelerating ALP. Techniques exist to accelerate sparse matrix computations using hypergraph partitioning, either on distributed-memory [13, 80, 57], shared-memory [83, 84], or both simultaneously [87, 85]. However, based on the computation, either the hypergraph representation of a sparse matrix must be adapted, the minimization objective modified, or both; see, e.g., Ballard et al. [5] who consider sparse matrix–matrix (SpMSpM) multiplication rather than sparse matrix–vector (SpMV) multiplication, as most preceding cited works. Thus for ALP as a programming model, the challenge lies in how these models and optimization techniques may be combined – preferably transparently to the programmer – to optimize the arbitrary sequences of computations and inputs that ALP encounters.

For example, while we may readily reuse known techniques to optimize any program consisting of SpMV multiplications with the same input matrix and some vector operations, the framework must be smart to select a different model and optimization objective when it concerns SpMSpM multiplication instead. Furthermore, relying on such existing work requires ALP to translate between different partitionings whenever differing operations or differing input matrices are encountered.

Ideally, however, the framework co-optimizes across multiple primitives and inputs that it encounters. The following avenues seem possible:

1. dynamically building fine-grained (hyper)DAG representations, followed by partitioning, (Hyper)DAG partitioning [50, 59], or scheduling (see also the related problem 5.2);
2. employing a coarse-grained parameterized representation of the computation and employing analytic choices, or
3. some mixture of the preceding avenues.

Difficulties with the first solution likely relate to the scale of the resulting optimization problem. For the second, while work in nonblocking ALP/GraphBLAS execution shows that such approaches may be effective [45], it is unclear how they may extend to arbitrary

primitives and inputs. A successful solution thus may well lie with the third option, and require mixed fine- and coarse-grained representations combined with both combinatorial and analytic techniques.

Sparse Matrix Partitioning

Given an $m \times n$ matrix A with N nonzeros, the sparse matrix partitioning problem seeks a partition of A into p disjoint parts $A = \cup_{i=0}^{p-1} A_i$ such that the number of nonzeros in part A_i satisfies $|A_i| \leq (1+\varepsilon) \left\lceil \frac{N}{p} \right\rceil$ for $0 \leq i < p$, where $\varepsilon \geq 0$ is a given load-imbalance parameter. Important questions for the area of sparse matrix partitioning as well as graph and hypergraph partitioning are: *How good is heuristic bipartitioning compared to exact bipartitioning? How good is recursive bipartitioning into k parts compared to direct k-way partitioning?*

To answer these questions, we can solve a set of small- and medium-size problem instances to optimality using an exact algorithm either based on the branch-and-bound (BB) approach, or on an integer linear programming (ILP) approach. To answer the first question, a set of 839 matrices has been bipartitioned by the programs MondriaanOpt [58] and MatrixPartioner [34]. To answer the second question, an exact bipartitioner has been employed within a recursive bipartitioning program for $k = 4$ and it has been compared with an exact direct 4-way partitioner using the program General Matrix Partitioner (GMP) [31] and the commercial ILP solver CPLEX.

We would like to scale up these initial results, to reach larger problems and be able to answer the main questions with more confidence. Since for $k = 2$ the bipartitioner MP works best, we ask whether its algorithm and implementation can be further improved. Parallelization should also help to enlarge our database of solved problems. One might interpret this database as a training set for learning (by either machines or humans) about properties of optimal solutions.

For $k > 2$, we surprisingly found that a basic formulation as an ILP solved by a commercial ILP solver was far superior to the BB solver GMP, and this poses the question what we can learn from the ILP solvers. Furthermore, can we use them for certain types of sparse matrix/graph partitioning? Finally, can we improve the basic formulation of the ILP to solve even larger problems?

Scalable Distributed Memory Partitioning

Scalability of high quality parallel (hyper)graph partitioning remains an active area of research. In particular, achieving good scalability and quality on large distributed memory machines is still a challenge, but even on shared-memory machines, scalability to a large number of threads seems difficult. Even more difficult is aligning the inherent complexity and irregularity of state-of-the-art algorithms with the restrictions of GPUs or SIMD instructions. Another conundrum is that, for good memory access locality during partitioning, (hyper)graphs need to already be partitioned reasonably well. Hierarchies of supercomputers have to be taken into account during partitioning. This can be done by using multi-recursive approaches taking the system hierarchy into account or by adapting the deep multilevel partitioning approach sketched above to the distributed memory case. When arriving at a compute-node level, additional techniques are necessary to employ the full capabilities of a parallel supercomputer. For example, many of those machines have GPUs on a node level. Recently, researchers started to develop partitioning algorithms that run on GPUs and, while of independent interest, partitioning algorithms developed for this type of hardware can help in that regard. Hence, future parallel algorithms have to compute partitions on and for

heterogeneous machines. On the other hand, algorithms should be energy-efficient and performance per watt has to be considered. Lastly, future hardware platforms have to be taken into consideration when developing such algorithms. One way to achieve this will be to use performance portable programming ecosystems like the Kokkos library [76].

Balanced Edge Partitioning for Distributed Graph Processing

The generally accepted formulation of the edge partitioning problem imposes a load balancing constraint on the number of *edges* per partition (cf., e.g., [47], [48]): $\forall p_i \in P : |p_i| \leq \alpha * \frac{|E|}{k}$ for a given $\alpha \geq 1, \alpha \in \mathcal{R}$, where $|p_i|$ denotes the number of edges in partition p_i. However, balancing only the number of edges does not always lead to good load balancing in distributed graph processing, as shown in [49]. In some cases, it is better to balance the number of vertex *replicas* – vertex copies produced whenever incident edges are placed in different partitions. The open problem is to achieve an edge partitioning that is balanced both in the number of edges and vertices while minimizing the vertex replication factor. First thoughts in that direction may lead to the formulation of a multi-constraint partitioning problem.

Provably Effective Graph/Hypergraph Coarsening

Today almost all of the state-of-the-art graph and hypergraph partitioning tools utilize multi-level approaches that are comprised of three phases: coarsening, initial partitioning and uncoarsening/refinement. Even though numerous different coarsening techniques have been proposed and many are shown to be effective in multi-level partitioning, we still do not have a provably effective and efficient coarsening technique for graph or hypergraph partitioning problems. The situation is more dire for directed graph and hypergraph partitioning for acyclic partitioning. Keeping acyclicity during coarsening is a desirable property, yet, it is computationally expensive to ensure and maintain acyclicity, with flexible coarsening techniques.

Today we also do not have a well-defined objective for coarsening. In other words, we do not have well-agreed upon desirable properties of the coarsened graph. Overall we want to solve a partitioning problem, but in multi-level partitioning the overall success of the algorithm is a complex function of the three phases of the multi-level approach. We have many counterexample results showing that the best initial partitioning solution does not always yield the best result. Hence, it is even more difficult to define a goal for coarsening.

In undirected graph and hypergraph partitioning, many successful tools use randomized heavy edge matching/clustering techniques, where vertices are visited in random order, and they are matched with their unmatched neighbor with the heaviest connection. This randomization helps to "maintain" the graph's structure. Hence, one potential direction for successful coarsening techniques is randomized algorithms (see Section 5.2).

Randomized Algorithms for Graph Sparsification and/or Coarsening

Randomized algorithms on networks often involve sampling nodes, edges, or subnetworks [24, 25, 35, 72]. These sampling techniques are used as subroutines (1) for the solution of fundamental problems on networks, such as connected components, the assignment problem, breadth-first search on long-diameter graphs, or global minimum cut, and (2) for graph learning problems trained with variants of mini-batch stochastic gradient. These problems are widely encountered in the US DOE applications, e.g., the use of the assignment problem in optimal transport (transforming probability distributions) for cosmology, the use of connected components in genomics problems. Sketching and sparsification, which are other randomization techniques used for networks, can be used to find approximate solutions

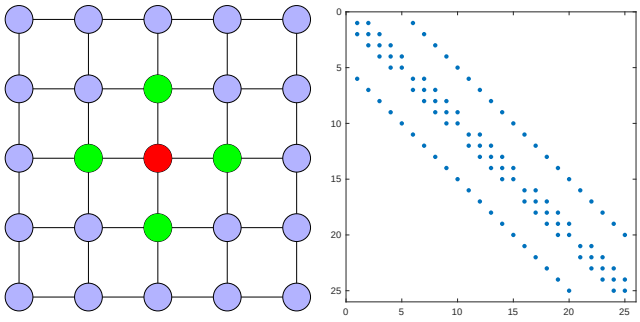

Figure 1 The 2D mesh resulting from the discretization of a square domain with the five-point stencil, using 5 points in each dimension, and the corresponding matrix after a row-by-row ordering of the mesh points. . Left: A 2D mesh. Right: The matrix of the mesh.

for higher-level problems where the network problem is a subroutine. The computational science applications include domain-decomposition solvers, iterative solvers, preconditioning for sparse systems using approximate factorization. Sampling and sketching can also be used as a coarsening technique in multilevel graph partitioning. Unfortunately, the impressive advances in the theory of randomized algorithms for networks has not been translated into practical demonstrations. There are ample research opportunities to bridge this gap between theory and practice, and hence, to produce high-quality software running on modern HPC hardware with demonstrations on application codes.

Balanced Streaming Partitioning

In streaming edge partitioning, edges are presented one at a time in a stream and must be assigned to a partition irrevocably at the moment they are encountered. Degree-based hashing has been proven effective for streaming edge partitioning, however, its potential benefits in the context of streaming *vertex* partitioning remain to be explored. An open problem is to investigate the benefits and challenges associated with using degree-based hashing techniques specifically for streaming vertex partitioning. Another notable limitation in the current literature on streaming partitioning algorithms is the predominant focus on common ordering strategies for the input (hyper)graph, such as random ordering, breadth-first search, and depth-first search orders. While these ordering strategies provide valuable insights into the performance of partitioning algorithms, they may not fully capture the challenges posed by real-world scenarios. Hence, it is an open problem to test streaming partitioning algorithms under adversarial node and edge orderings, particularly in the context of buffered streaming algorithms, where locality has a large impact on the quality of the result.

An open problem in the field of streaming process mapping is to address the problem when the underlying topology cannot be faithfully represented as a hierarchy, but only as a graph or hypergraph. Existing streaming algorithms either ignore the topology, i.e., solve the graph partitioning problem, or optimize directly for hierarchical topologies. However, many real-world scenarios involve complex interconnections that form graph-based topologies.

Exact Solvers for Large k (Hyper)graph Decomposition

Solving the graph bipartitioning problem to optimality using branch-and-bound algorithms has recently been shown to be highly effective if the optimum solution value is very small. For example, Delling et al. [20] can solve instances with millions of vertices to optimality in

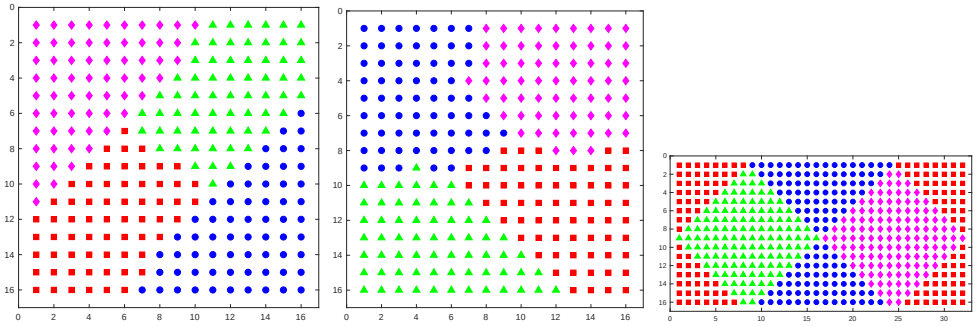

Figure 2 Partitioning the 16×16 mesh with different routines; the basic diamonds cannot partition this mesh, but can partition a larger one. Left: The $K = 4$-way partition of the 16×16 obtained by the special routines [26]. Connectivity-1 is 58. Middle: The $K = 4$-way partition of the 16×16 mesh obtained by PaToH, suboptimal (connectivity-1 is 61). Right: The $K = 4$-way partition of the 16×32 mesh by the basic diamonds [8, Section 4.8], which is believed to be asymptotically optimal. Here though the connectivity-1 is 126 and PaToH obtains 93.

a reasonable amount of time. It is still open whether such solvers also exist for balanced (hyper)graph partitioning problems where k is significantly larger than 2. The difficulty here comes from the fact that larger values of k introduce a large amount of symmetry in the problem, i.e., if you have some partition of the graph, then any permutation of the block ids is also a partition of the graph that has the same balance and objective. Another problem of current solvers is how to handle dense instances or, more precisely, instances in which the objective function is large.

Partitioning Stencils and Analyzing The Performance of Partitioning Tools

We investigate the scalability of the graph- and hypergraph-based sparse matrix partitioning methods in terms of being able to obtain high quality solutions in large problem instances. The quality measure that we are interested is the connectivity-1 metric, which usually measures the total volume of communication when vertices represent data items/computations and the hyperedges represent the dependencies. Ideally, theoretical investigations help explain the scalability or success of the methods. However, the current algorithms in use are too sophisticated to lend themselves to such an approach. We are thus looking for sound experimental methodology.

One approach is to take a subclass of problems, develop special partitioners, and compare the hypergraph partitioners with those. We take five-point stencil computations in two-dimensions (2D) for which we have a special linear-time partitioner [26, 77] and see how good the current partitioning methods are on these cases. We compare the performance of hypergraph partitioners on these. A rectangular 2D domain is discretized with the five point stencil and a mesh of size $X \times Y$ is obtained whose points are placed at integer locations. Two points (x_1, y_1) and (x_2, y_2) of the resulting mesh are neighbors iff $|x_1 - x_2| + |y_1 - y_2| = 1$. A sample mesh resulting from the discretization of a square domain with five points in each dimension is shown in Figure 1. The figure also shows the connections of a point. After an ordering of the mesh points, one can obtain an $X^2 \times Y^2$ matrix. The matrix obtained from the shown mesh after a row-major ordering is shown in Figure 1.

A partitioning of the points of the mesh $\mathcal{M}$ corresponds to a row-wise or a column-wise partitioning of the associated matrix $\mathbf{A}_{\mathcal{M}}$. Without loss of generality let us focus on the row-wise partitionings of $\mathbf{A}_{\mathcal{M}}$. The standard column-net hypergraph $\mathcal{H}_{CN}$ model [11] can

Table 1 The partitioning of the $X \times X$ mesh of five-point stencils with perfect balance using the method of Grandjean and Uçar [26] obtains the numbers given in row "Vol" as connectivity−1 metric of the cut. PaToH's results are in the row "PaToH" – they do not have perfect balance. Apart from 58 in the last line, the other numbers are claimed to be optimal.

X	16	64	256	1024	2048
PaToH	61	249	985	4034	7999
Vol	58	222	878	3500	6996

be used for this purpose. Partitioning the vertices of the hypergraph $\mathcal{H}_{CN}$ among K parts will therefore correspond to partitioning the stencil computations among K processors; the connectivity−1 metric of the cut will measure the total communication volume; and the balance of part weights in terms of vertices will correspond to balance of the loads of the processors. We assume unit vertex weights here, the effect of having less operations on the border points of the mesh will be ignored for simplicity (and is negligible).

With the special partitioning methods by Grandjean and Uçar, we obtain the total communication volume listed in Table 1. While the communication volume listed in the table is obtained with the routine itself, we note that it is given by the formula

$$2 \times \left(\left\lfloor \frac{n}{\sqrt{2}} \right\rfloor + n \right) + 4 \,, \tag{1}$$

which is claimed to be optimal for $X > 16$ in the table (for $X = 16$, the optimal communication volume is claimed to be 57).

This formula requires some conditions on X, which we do not give here. Are the connectivity−1 values given in Table 1 optimal for a perfectly balanced 4-way partitioning of the two mesh of $X \times X$ points discretizing a square domain with a five point stencil? For the 16×16 mesh, Gurobi solver [28] also finds a cut of value 57 in a few minutes under an additional constraint to assign the four corners to four different parts). The solution obtained by the Gurobi solver is at the close neighborhood of what is shown in Figure 2; by the method of Grandjean and Uçar is easily updated to mimic Gurobi's result.

Another point that arise from the given 4-way partitioning is that these partitions cannot be obtained in a recursive bisubsection scheme where each step greedily optimizes the cut hyperedges with perfect balance. This is so, as the first cut vertically cuts the mesh into two equally sized parts with perfect balance and optimal cut. Simon and Teng [70] delve more into this point in the context of graph partitioning.

We note that more results of the sort are given elsewhere [26]. The same reference also surveys some results from the literature, including references on discrete isoperimetric problems [81], which can be used to guide algorithms. Two things are of particular note: in the corners, the optimal parts are triangle-like, as in two corners in Figure 2 (left), and in the interior the optimal parts are diamond-like as in Figure 2 (right).

Bisseling and McColl [9] propose digital diamonds to partition similar meshes with wrap-around connections. Digital diamonds are ℓ_1-spheres defined with a center (c_x, c_y) and a radius ρ. Such a diamond contains all mesh points (p_x, p_y) where with $|p_x - c_y| + |p_y - c_y| \leq \rho$. Grandjean and Uçar give formulas for the total communication volume when one uses digital diamonds. They also specify conditions on mesh and part sizes under which a partition by digital diamonds are possible. Basic diamonds proposed by Bisseling [8, Section 4.8] trim off two borders from the digital diamonds to address partitioning of another set of mesh and part sizes – these conditions as well as the total volume of communication are also specified by Grandjean and Uçar. Digital diamonds and basic diamonds are believed to be

asymptotically optimal in terms of the total communication volume, but obtain disconnected partitions on the borders of the mesh when there are no round-around connections – which is not desirable in certain applications.

Another approach is to take general sparse matrices boost the data in a way, reason about it and evaluate the performance of hypergraph partitioners on these. For example, suppose we partition a matrix A row-wise into k parts, and obtain a total communication volume of T_V units in SpMxV. Then, if we partition the matrix $B = [A, A]$ row-wise again into k parts, then the first partition should be good for B with $2 \times T_V$ communication volume. If our partitioning tool is good, such a performance is expected; if the answers were not T_V vs $2 \times T_V$, we could either improve the partition of A or B. Similarly, a k-way row-wise partition of $C = [A; A]$ – this time two copies of A are stacked to have twice as many rows – should have a communication volume of T_V units. Some experimental investigation with PaToH [12] using these matrix repetition schemes [77] reveals a good behavior. What else can we say about the behavior of partitioning tools on more general problems?

Highly Spread Out Weights in Mesh Partitioning

Many distributed numerical simulations rely on mesh partitioning to improve the balance of their computations on every computing unit, thus increasing their efficiency and scalability. A mesh is modeled by its dual graph or hypergraph as input to a partitioner: each vertex corresponds to a cell of the mesh, and the vertex weight is the computing cost of this cell. Good quality hexahedral meshes have a reasonably regular topology, mostly looking like a 2D or 3D grid. However, the vertex weight distribution can be highly spread out for various applications like Monte-Carlo particle transport simulations. For this kind of instance, classic multi-level approaches of the existing graph partitioner can have some quality issues, symmetric to the ones observed in Section 5.2. Multi-level graph partitioners focus on topological properties, and here, taking more into account vertex weight distribution should lead to better and faster obtained partitions.

Cartesian Mesh Partitioning

Directly addressing data in memory is crucial in achieving high performance when running on modern architectures, especially on GPU. Grids allow direct access to neighbor cells for mesh computations, making stencil computations like the one presented in Section 5.2 very efficient. However, standard partitioning approaches lead to non-rectangular parts, making distributed applications less efficient. Thus, a new problem is partitioning a grid into parts that are all a subgrid or a set of subgrids. Such a partitioning model will also work to partition block structured meshes that often arise for hexahedral meshes.

Problems in Multilevel Graph Partitioning With Star Graphs

The partitioning community has long focused on instances with a regular structure, e.g., mesh graphs or instances from circuit design. However, it becomes more and more important to find high-quality solutions for instances with an irregular structure, such as those derived from social networks. Surprisingly, we found a subclass of these instances where current state-of-the-art partitioning algorithms compute solutions that are far from optimal. The identified instances – referred to as *star instances* – are characterized by a core of a few highly-connected nodes (core nodes) with only sparse connections to the remaining nodes (peripheral nodes). One example of such an instance is the Twitter graph. Here, we found that partitioning the nodes into low- and high-degree vertices ($\leq$ median degree)

induces a bipartition that cuts half the edges as any of the existing multilevel partitioning tools. We identified several other social networks where we observed the same behavior. Thus, it becomes increasingly important to develop efficient partitioning techniques that can handle such instances. From a theoretical perspective, we were already able to present an $(R+1)$-approximation for star instances, where R is the ratio of an approximation algorithm for the min-knapsack problem. This is a remarkable result since there exists no constant factor approximation for the general graph partitioning problem.

Graph Partitioning with Ranked Vertices

For some graph algorithms, there is an implicit rank over the vertices. For instance, 2-hop indexing generates a *label cover* that can be used for answering pairwise shortest-distance queries. Classical algorithms, e.g., Pruned Landmark Labeling (PLL) [1] and its variants, leverage a ranking that has a drastic impact on the number of entries stored at local vertex indexes. In the distributed setting, the amount of entries in the *cut*, i.e., the ones replicated and/or communicated among the nodes, depends on this ranking. Especially when the number of nodes is high, this communication can create a bottleneck. For distributed execution, ranking the vertices also changes the loads on each part. In that sense, another problem at hand is given the rank, the amount of data stored at each vertex needs to be estimated well enough so that the part weights incur an acceptable level of imbalance. Hence, the problem is given a graph $G = (V, E)$, *what is the best vertex ranking and partitioning pair that yields the best performance in terms of execution time and maximum memory used at each node?*

Designing Multilevel Algorithms

In a variety of fields, computational optimization challenges often arise when modeling large and complex systems, presenting significant hurdles for solving algorithms, even when high-performance computing resources are deployed. These obstacles are frequently due to a multitude of factors such as an extensive number of variables and the complexity in describing each variable or interaction. Problems involving combinatorial and mixed-integer optimization add extra layers of complexity. Specifically, the presence of integer variables frequently results in NP-hard problems, particularly in contexts where nonlinearity and nonconvexity are factors.

A widely adopted strategy for tackling these challenges involves the use of iterative algorithms. While these algorithms may be grounded in divergent algorithmic paradigms, they often exhibit a similar pattern: rapid improvement during initial iterations followed by a phase of slower progress. In the realm of iterative algorithms, utilizing first-order optimization techniques like gradient descent or methods that rely on limited observable data, such as local search, often leads to a local optimum that is usually suboptimal when compared to the true global optimum. Additionally, the algorithms employed within each iterative cycle are not always exact, further complicating the optimization process. To speed up these algorithms at each iterative step, various strategies including heuristics, parallelization, and different ad hoc techniques are commonly employed, albeit often at the expense of solution quality. Being trapped in local optimum of unacceptable quality is one of the most important issues of such algorithms.

Multilevel methodologies have been introduced to address the challenges of large-scale optimization, offering a strategy that reduces the chances of being trapped in low-quality local optimum. These techniques are complementary to stochastic and multistart approaches, which

also help the algorithm escape local optima. While there's no one-size-fits-all prescription for designing multilevel algorithms, their core philosophy revolves around global considerations while executing local actions based on a hierarchy of increasingly simplified representations of the original complex problem.

In practice, a multilevel algorithm initiates the optimization process by generating a hierarchy of progressively simplified (or coarser) problem representations. Each subsequent coarser level aims to approximate the problem at the current level but with fewer degrees of freedom, facilitating a more efficient solution process. After solving the coarsest problem, its solution is extrapolated back to the more detailed level for further refinement – a phase termed as "uncoarsening." Employing this multilevel approach frequently results in substantial improvements in both computational efficiency and the quality of solutions. There are many broad impact open questions in designing multilevel algorithms for (hyper)graphs some of which we mention here.

Distance between vertices. In order to coarsen the problem, a critical issue is to design a distance (or similarity) function between nodes. The question is simple: how to introduce a similarity function that will effectively find subsets of nodes that share the same solution (e.g., in the context of graph partitioning it is about predicting that nodes will be assigned the same part)? Incorrectly chosen subsets of nodes will mislead coarsening and will make the uncoarsening to work much harder which will result in increased complexity and poor results. In the same time, sophisticated distance functions are not supposed to destroy the overall complexity of the multilevel algorithm. Examples of such advanced solutions are spectral-based [16, 61, 69] and low-dimensional representations [73]. They work very well on the partitioning, ordering [66] and clustering multilevel schemes. However, there is also a lot of evidence that these algorithms are not perfect and do not fit all scenarios.

Density of coarse levels. This remains one of the most crucial issues in multilevel algorithms. In many problems and coarsening schemes the more we coarsen the problem, the more dense graphs are obtained unless we deliberately take actions to sparsify them. On the one hand, such dense representations often may approximate the original problem better. On the other hand, the complexity of refinement at the corresponding levels of uncoarsening becomes prohibitive. For example, in the algebraic multigrid inspired multilevel approach for graph linear ordering this issue was simply patched by reducing the interpolation order [64] which is a pretty blind solution. It was slightly improved in graph partitioning [65] by using a better node distance function in combination with the small interpolation order but more sophisticated and theory-grounded approaches are required. In a similar 2-dimensional layout problem, the authors switched to more regular coarsening with the geometric multigrid [60]. In general, dense graphs are problematic for most existing multilevel algorithms that mostly designed for sparse instances and require special treatment such as other coarsening schemes or special hardware [43].

Maximization problems. A particularly interesting class of problems for which multilevel algorithms have not reached their advanced stage is maximization problems such as max cut, maximum independent set, and maximum dominating set. A traditional coarsening approach quickly generates dense coarse levels and becomes impractical. Recent work on sophisticated node distance functions and sparsification improve the situation [3] but after a certain number of levels the quality of coarse levels becomes either poor (if sparsified) or intractable (otherwise). Rethinking of the coarsening ideas is required for this class of problems as such approaches as inverting graphs quickly become impractical.

When to stop the refinement? Perhaps there is no multilevel algorithm whose developers have not asked this question. Overall, there is no theory-grounded work related to optimization on (hyper)graphs that answers this question. Apart from the complexity issue, on the first glance it may look trivial that in the ideal refinement, the employed local optimization solvers should be optimal. However, there is a lot of practical evidence that terminating refinement before reaching the best possible local solution is beneficial to the final global suboptimal solution.

Advanced types of multilevel cycles. In multilevel schemes, the V-cycle coarsening-uncoarsening is the most basic and widely used cycle for this purpose, but several other advanced cycles aim to improve the efficiency and effectiveness of multilevel methods. Most widely used of them are: (1) the W-cycle is a more advanced version of the V-cycle that provides a more aggressive approach to solving the coarser problems. In a W-cycle, a refinement and full deeper W-cycle is performed at each coarser level before moving back to the finer level. This allows for more thorough refinement at lower levels, often leading to better convergence properties compared to the V-cycle. (2) The F-cycle method creates the hierarchy of coarse representations and starts at the coarsest level and works its way up to the finest grid, solving the problem at each level by applying another full V- or W-cycle. It combines with V-cycles or W-cycles at each level for better optimization of coarse levels. Both F- and W-cycles are particularly effective for problems where an initial coarse approximation is not easy to obtain. Both cycles usually exhibit better then in V-cycle quality which comes at additional cost of complexity. The W-cycles are usually more expensive but do exhibit a good quality [62, 63]. Finding robust criteria on when to recursively apply one or another type of advanced cycle (if at all) is very important in multilevel algorithms as their running time is increased with the advanced cycles.

5.3 (Hyper)graph Clustering

Correlation Clustering

In the correlation clustering problem the input is a graph with edges labeled with + and − (or simply with +1 and −1). + indicates that the endpoints of the edge should be in the same cluster, and − means that the endpoints of the edge should be in different clusters. The goal of correlation clustering is to find a clustering that respects as many of these requirements as possible. Of course respecting all of them is in general not possible, and so a commonly studied objective is to minimize the number of disagreements.

There is a big discrepancy between the theory work on correlation clustering and what is done in practical solutions. For example, while the famous PIVOT algorithm provides 3-approximation for complete graphs, if the algorithm is run on a sparse graph (i.e., one where + edges induce a sparse graph) the algorithm often gives a solution that is worse than leaving each node in a cluster of size 1. Better approximation algorithms are known, but they are not as scalable, as they rely on solving an LP or SDP. In the case of weighted or not-complete graphs the best known approximation ratio is $O(\log n)$.

Despite all of these theoretical advances, the solutions that are implemented in practice are based on local swaps and a multilevel approach. In particular, the basic operation that these algorithms make is moving a node to a neighboring cluster, only if this increases the overall objective. This way, the algorithm essentially treats the objective function as a blackbox and does not leverage all the structural properties of the problem, which are used to give approximation algorithms.

While the practical implementations are quite scalable, there is probably room for improvement, as the number of logical rounds needed to obtain a good solution goes in hundreds. This in particular makes these algorithms not easy to use in distributed settings.

An interesting open problem is to bridge the gap between theory and practice for correlation clustering with the goal of obtaining better practical implementations. Specifically, it would be interesting to develop algorithms requiring fewer rounds, which will make them amenable to an efficient distributed implementation.

Overlapping Edge-Colored Clustering

Edge-Colored Clustering is a categorical clustering framework [2] whose input is an edge-colored hypergraph and output is an assignment of colors to nodes which minimizes the number of edges where any vertex has a color different from its own (*mistakes*). We are interested in variants of this problem which allow budgeted overlap. Specifically, the following three notions were defined in [17]. LocalECC allows up to b of color assignments at each node. GlobalECC allows one "free" color assignment for each node, plus b additional assignments across all nodes. RobustECC allows each node to either receive exactly 1 color, except that at most b nodes are assigned *every* color. Equivalently, at most b nodes are deleted.

Each of these problems generalizes ECC, with equivalence for the first coming at $b = 1$ and for the latter two at $b = 0$. Consequently, they are each NP-hard (Angel et al. [2]). We (Crane et al. [17]) showed that greedy algorithms give an r-approximation on the number of edge mistakes, where r is the maximum hyperedge size. Further, for LocalECC, a $(b + 1)$-approximation can be achieved with LP-rounding. More generally, we ask about bicriteria (α, β)-approximations, where α is the approximation factor on edge mistakes and β is the approximation factor on the budget b, and show that all three variants have such approximation algorithms, though the factors are no longer constants for GlobalECC.

Open Problems. Are these ideas relevant for any practical applications? Where? What can we assume about the inputs in those settings? Are there constant-factor single-criteria approximations for the Global and Robust versions? Does GlobalECC have a constant-constant bicriteria approximation? More generally, bicriteria inapproximability is an interesting and relatively unexplored direction. We saw that empirically these approximations performed much better in practice than the guarantees. Is there some sort of structure in real-world instances that we can model to improve our analysis?

Dense Graph Partition

Dense Graph Partition, introduced by Darley et al. [19], models finding a community structure in a social network. Formally, given an undirected graph $G = (V, E)$, the task is finding a partition $\mathcal{P} = \{P_1, \ldots, P_k\}$ of V, for some $k \geq 1$, of maximum density. With $E(P_i)$ denoting the number of edges among vertices in P_i, the density of $\mathcal{P}$ given by $d(\mathcal{P}) = \sum_{i=1}^{k} \frac{|E(P_i)|}{|P_i|}$. Note that there is no restriction on the number of communities which yields some difference to the problem of partitioning into cliques. While there exists a partition into exactly k sets of density $(n - k)/2$ if and only if the input graph can be partitioned into k cliques [6], there can be a partition into less than k sets with a density higher than $(n-k)/2$ even if the input cannot be partitioned into k cliques. Alternatively, Dense Graph Partition can be modeled from a game theoretic perspective. Aziz et al. [4] study the Max Utilitarian Welfare problem where the vertices in a graph $G = (V, E)$ are agents, and each agent $x \in V$ validates its coalition $P \subseteq V$ with $x \in P$ by $\frac{1}{|P|}|\{u \in P \mid \{u, v\} \in E\}|$. Maximizing social welfare for this model is equivalent to Dense Graph Partition.

It is known that maximum matching is a 2-approximation [4], and there are a few improvements on specific graph classes: polynomial-time solvability on trees [19], $\frac{4}{3}$-approximation on maximum degree 3 graphs, and EPTAS for everywhere dense graphs [6]. This in particular gives rise to the questions: Can the 2-approximation be improved, at least on some more non-trivial graph classes? Does there exist a polynomial-time approximation scheme on general instances? Is it true that there is always an optimum solution where all parts induce a graph of diameter at most 2, a so-called *2-club clustering*? What is the complexity on graphs of bounded treewidth?

Streaming Graph Clustering

Streaming Graph Clustering is commonly defined as follows: given a graph $G = (V, E)$, find a clustering $\mathcal{C} : V \to \mathcal{N}$ that maximizes a quality score such as modularity, using at most $O(|V|)$ memory. In the one-pass version, E is an ordered list of edges and each edge can be read only once. A popular heuristic for this problem is SCoDA [29].

This matches well with real-world applications where graphs are discovered over time, e.g. in online social networks, as well as for graphs which are too large to cluster using standard $O(|E|)$ memory algorithms. However, the one-pass version is quite limiting and often results in low clustering quality [38].

The Incremental Graph Clustering model [38] is a *buffered* variant of the one-pass model where the ordered edge list is subdivided into *batches*. Unlike in buffered streaming graph partitioning [21], the batches are assumed to be given and not selected by the algorithm. Edges in a batch are read and processed in memory together. The algorithm can use $O(|E|)$ memory, but we require that running time for processing each batch does not depend on $|E|$, only on the size of the batch.

The Neighborhood-to-community link counting (NCLiC) [38] is a heuristic for this variant. For modularity clustering, it provides strong modularity retention compared to offline algorithms. It applies the Leiden Algorithm to each new batch and then merges it with the already processed graph.

Open Problems. The NCLiC algorithm keeps track of the approximate number of neighbors in each cluster. If a vertex changes community it will update its neighbors with a probability that depends on its degree. Skipping some updates allows maintaining the required running time, but introduces a reduction in clustering quality. Is there a data structure that allows keeping exact counts of the neighboring clusters without violating the running time constraint?

Another open question is: is it possible to modify NCLiC to use at most $O(|V|)$ memory while retaining most of the modularity retention qualities?

5.4 Data Reductions and Learning

Data Reductions for (Hyper)Graph Decomposition

Most balanced (hyper)graph partitioning formulations are NP-hard: it is believed that no polynomial-time algorithm exists that always finds an optimal solution. However, many NP-hard problems have been shown to be fixed-parameter tractable (FPT): large inputs can be solved efficiently and provably optimally, as long as some problem parameter is small. Over the last two decades, significant advances have been made in the design and analysis of fixed-parameter algorithms for a wide variety of graph-theoretic problems. Moreover, in recent years a range of methods from the area have been shown to improve implementations

drastically. For example for the maximum (weight) independent set problem [27]. Here, data reductions rules transform the input into a smaller one that still contains enough information to be able to recover the optimum solution. For the maximum independent set problem, this enabled highly scalable exact solvers that can solve instances with millions of vertices to optimality. For balanced partitioning this has currently not been carefully investigated. However, here are some very simple data reduction rules. For example, removing a vertex of degree one, then solving the smaller subproblem with same balance constraint and afterwards assigning the vertex to a block with leftover capacity, is a valid data reductions rule. This yields the natural open questions: are there more and highly effective data reduction rules for balanced (hyper)graph partitioning problems? These rules could be helpful in two ways: they could speedup current heuristic solvers, e.g. multilevel (hyper)graph partitioning algorithms, and they could help to build more scalable exact partitioning algorithms (see Section 5.2).

After all reduction rules for kernel computations have been applied, the final smaller instance can still be too large to be solved to optimality within a reasonable time bound. This is a serious problem as the overall goal of the algorithms is to solve the given problem instance. The idea of lossy kernelization is as follows: when no more reductions can be applied, i.e. a problem core has been computed, one may shrink the input further while guaranteeing that the optimal solution value changes only slightly. Then a good approximate solution of the reduced input can be lifted to a good approximate solution of the original input. This has recently been done for the vertex cover problem [40]. The natural question that arises is can these techniques be applied to balanced (hyper)graph partitioning as well?

As the (lossy) kernel/core still contains the optimum solution (or some approximation thereof) in some sense, this has a large potential to speed up the (multilevel) heuristic while not sacrificing solution quality. Additionally, running a fast algorithm on the large kernel can help to identify parts of the instances that are likely to be in a good solution. Those parts can then be put into a partial solution and the remaining instance can be reduced recursively.

It could also be possible to use machine learning to learn lossy reductions for a wide-range of problems in this area. For example, one could use learning to predict if two vertices should be clustered together or to decide if an edge is a cut edge or not. The basic idea is then to use a classification model to learn which parts of the input can be pruned, i.e. are unlikely or highly likely in an optimum solution. In the first case, a solution omits this part of the input, in the latter case this part of the input will be included in the solution. For example, [39] propose to use machine learning frameworks to automatically learn lossy reductions for the maximum clique enumeration problem and [74] shows that this learning-to-prune framework is effective on a range of other combinatorial optimization problems. The classification model can be a deep neural network in an end-to-end framework or a classifier with significantly fewer parameters such as SVM or random forest if a deeper integration of machine learning and algorithmic techniques is done. The latter will require carefully engineered features based on existing heuristics.

Learning for Local Search in Multi-level (Hyper)graph Partitioners

Machine learning techniques can also be used to learn more efficient refinement steps. Existing refinement steps in multi-level graph partitioning techniques rely on solving a flow problem or iterative moves of Kernighan–Lin or Fiduccia–Mattheyses heuristic. However, solving flow problems can be quite slow (given the number of times it is called). Similarly, the number of possible moves that need to be explored for finding a good step using Kernighan–Lin or Fiduccia–Mattheyses can be quite high. It is worthwhile exploring if learning techniques can be used to predict good regions where the flow algorithm can focus. This can improve the

trade-off between the time to solve the flow problem and the gain from it for the refinement part. For the case of the Kernighan–Lin or Fiduccia–Mattheyses heuristic, the interesting question is whether learning techniques such as reinforcement learning can be used to learn a good sequence of moves for these local search heuristics. This has the potential to reduce the search space that needs to be explored to find good local moves. For training the learning techniques, the R-MAT graph generator from the Graph500 benchmark can be used.

5.5 Embeddings

Distance Estimation for Process Mapping

Process mapping is a super-problem of graph partitioning, in which vertices of some source graph S have to be assigned (i.e., mapped) to vertices of some target graph T, by way of a mapping function $\tau_{S,T} : V(S) \longrightarrow V(T)$, so that an objective function is minimized. In the field of parallel computing, source graphs commonly represent computations to be performed, usually multiple times in sequence, while target graphs represent processing elements and interconnection networks of multi-processor and/or multi-computer hardware architectures. The objective function to minimize is the amount of data to be exchanged across the interconnection network, so as to reduce its congestion, provided that every processing element in $V(T)$ receives roughly the same number of vertices of S (or, more generally, equivalent vertex weights with respect to its compute power), to minimize computation imbalance. In this context, partitioning some graph S into k parts amounts to mapping S onto $K(k)$, the complete graph of order k, since in this case all processing elements are at the same distance from all the others.

In the Dual Recursive Bipartitioning (DRB) algorithm [54] used by the Scotch software, computing the mapping of S onto T requires to be able to estimate the shortest-path distance in T between any two vertex subsets of $V(T)$ called the *subdomains* of $V(T)$. These subdomains are not arbitrary, since they result from recursively bipartitioning the graph T into pieces of roughly the same size in a way that minimizes the cut of the interconnection network. Being able to compute the distance between any two subdomains allows the DRB algorithm to estimate the penalty of assigning some vertex v of S to either one of two sibling subdomains of T, by estimating the distance between these subdomains and those to which all the neighbor vertices v of u have already been mapped. When the recursive bipartitioning of T is perfectly balanced, the number of subdomains of T is $2|V(t)| - 1$.

A way to quickly obtain the distance between any two subdomains of some target graph T is to pre-compute a distance matrix between all of them, of a size in $O(|V(T)|^2)$. While this solution works for small target graphs, it is no longer applicable when mapping onto big parts of very big target architectures. To solve this problem, one has to find a more compact (in terms of data storage) and quick (in terms of retrieval time) method to produce these distance estimates. An important condition on these approximations is that distances should become more accurate as subdomains are smaller and closer to each other in T.

In [55, 56], it has been shown that, for target architectures for which the recursive bipartitioning of subdomains, and the distances between subdomains, can be computed algorithmically, by way of explicit functions (e.g. , for regular vendor architectures such as meshes, butterfly graphs, etc.), a bipartition tree, created by way of recursive matching and coarsening of the whole target graph, allows one to represent any subset, even disconnected, of the processing elements of these target architectures. The DRB algorithm can therefore be applied to them.

However, for irregular architectures (e.g. , those represented by irregular graphs), the question remains open. It can be expressed in the following form: "How can one get cheaply (both in terms of memory and computation time) approximate distances between any pair of the subgraphs yielded by the recursive bipartition of some irregular graph?"

Space-Efficient Planar Graph Embedding

When one opens up a publication regarding planar graph bisubsections, one often reads a sentence akin to: Without loss of generality, assume that the input graph is embedded in the plane and maximal planar. Famous works that makes use of this specific property is the balanced separator theorem due to Lipton et al. [42], which states that every planar graph has a balanced vertex separator of size $O(\sqrt{n})$. Standard recursive bisubsection algorithms for planar graphs are based on this theorem, which are able to construct the entire recursive bisubsection in linear time [33]. Often it is easy to assume such an embedding, as it can be computed in linear time using $O(n \log n)$ bits of space, i.e., a linear number of words. In sub-linear space settings one can compute an embedding in polynomial time (albeit with an extremely large polynomial degree). Now, the question remains: what can one achieve when aiming for a linear time algorithm, while using $o(n \log n)$ bits, or ideally, $O(n)$ bits? The standard linear time algorithms are quite involved, but on the most basic level many of them use a simple depth-first tree and compute a constant number of, but seemingly critical, variables per vertex. Even when aiming for a much lower goal: check if the input graph is planar within $O(n \log n)$ time while using $o(n \log n)$ bits, there is no obvious way to tackle this problem. As graphs grow larger and larger, such questions of space-efficiency become of higher interest. Especially with the direct application of graph partitioning algorithms that rely on such embeddings.

Finding Moore-Bound-Efficient Diameter-3 Graphs

In graph theory, given a graph with degree d and diameter k, the largest number of vertices in that graph can be determined using the Moore bound. Recent technological advances in photonics technology have greatly increased the number of links – or degree d – of the network routers, improving the scalability of large supercomputers. While Moore-bound-optimal diameter-2 graphs have recently been engineered to span a few thousand nodes [36], emerging AI and graph applications are demanding larger configurations. Unfortunately, diameter-3 graphs are still elusive, with Moore's bound efficiencies of only 15%. The construction of more efficient diameter-3 graphs would directly impact the design of emerging photonics systems for large scale graphs [36, 37], data analysis, and AI applications.

5.6 Parameterized Complexity

Parameterized Complexity of Layered Giant Graph Decomposition

Direction 1. An important theme – or challenge – for theoretical computer science, that has been recognized for decades, is the observation that has been made prominently by Richard Karp and others that we don't really understand very well natural input distributions. *It is remarkable how well sometimes very simple heuristics work in practice for problems that are known to be NP-hard.* There must be some sort of structure, but what is it? And if we knew, could we exploit that in designing algorithms?

A striking example of this was described by Karsten Weihe in an old paper entitled, "On the Differences Between Practical and Applied" which was about Weihe's experience doing quite practical computing for a simple Hitting Set application in real-world computing where his project was tasked with computing a minimum number of stations that could service all of the trains of Germany.

The model is a straightforward bipartite graph, with trains on one side, and stations on the other, and an edge if a train t stops at a station s. There are two simple pre-processing vertex deletion rules: (1) If $N(s)$ is a subset of $N(s')$, then delete s. (2) If $N(t)$ is a subset of $N(t')$ then delete t'. Weihe found that these two simple reduction rules cascade back-and–forth on the gigantic real-world train graphs, and one ends up with (using PC terminology) a kernelized instance that consists of disjoint connected components that have size at most around 50, so the problem can be solved optimally by analyzing the connected components separately.

From the standpoint of parameterized complexity theory, we could simply declare the structural parameter of interest to be: k ="the maximum connected component size of the network G' that results when opportunities to apply the two reduction rules have been exhausted". This would be perfectly legal in the mathematical framework of PC – we could call the parameter the Weihe-width of the Hitting Set instance and have a pretty good FPT algorithm for computing what we could call a Weihe-width decomposition. This is legal, but from a traditional parameterized algorithms and complexity perspective, not entirely satisfying.

At the expense of quadratic blowup one can combinatorially reduce the very important medical- and bio-informatics problem of Feature Selection to Hitting Set in the following natural way. We now have enormous amounts of information concerning the genes that are being expressed into RNA, and so each patient in our hypothetical hospital has a gene activation profile. And each patient either does, or does not, have cancer.

We want to know a small subset of the genes to pay attention to so that we can accurately predict the outcome. On the one side, we have a vertex for each pair of patients that have differing outcomes, and on the other side, we have one vertex for each gene. It is surprising that Weihe's two reduction rules work quite practicably, in this very different real-world large data context. What is going on, and how can we generalize?

Open Problem. Can a Weihe-width k decomposition of a graph of size n be computed in truly linear FPT time?

A second open problem begins by reconsidering the most central example of an FPT graph problem, Vertex Cover, that has inspired in various ways a surprising amount of theoretical work in the parameterized complexity research community. For example, the recent work reported at IJCAI 2020 on the parameterized complexity *paradigm of solution diversity* began with an initial FPT result about the naturally parameterized Diverse Vertex Cover problem.

A (parameterized) vertex cover of a graph is a set of k vertices V' of $G = (V, E)$ such that the largest connected component of $G' = G - V'$ is size one! In other words, deleting the vertices of V' kills off all the edges of G, yielding, if we want to call it that, a very nice decomposition of G' into clusters of extremely high data-integrity and coherence, as each connected component consists of a single vertex.

It might seem that the Vertex Cover problem is so simple that it might be irrelevant for giant graphs. But by setting thresholds for declaring edges, it has been used very effectively in stages in very large dataset bioinformatics, e.g., Dehne's CLUSTAL W package for multiple sequence alignment [15].

A key point is that the successful CLUSTAL W algorithm begins by decomposing a sparse graph constructed by making edges between vertices (data objects) that are emphatically NOT similar. The impulse would be to seek cliques of compatible vertices, but here is exploited that the naturally parameterized Clique and Vertex Cover problems are parametrically dual, and from that point the CLUSTAL W algorithm proceeds in stages with an initial decomposition based on a vertex cover cutset on a sparse graph based on thresholding the NOT similarity that makes an edge in the initial graph.

The following problem explores a generalization where the resulting connected components ("clusters") satisfy other simple integrity requirements. It is called *Vertex Decomposition into Small Dominator Clusters*: given a graph $G = (V, E)$. and parameter (k, d), the question is can we delete k vertices from G, obtaining G' such that every connected component of G' has domination number at most d? It is interesting to start by asking if this might be FPT for the vector parameter (k, d). But, if we fix $k = 0$, then the problem is W[2] - complete. We can still hope for a parameterized tractability result, where d is allowed to play an XP-role in the exponent of the polynomial and for fixed d, with parameter k we get FPT.

Open Problem. Is this FPT? And if so, can the corresponding decomposition be computed in truly linear FPT time for $d = 1$?

Note that we could define endlessly many interesting and largely unexplored parameterized problems in a similar manner where the decomposition is modeled by connected components formed by essentially a cutset. And there is also the possibility of interestingly layered decompositions of this kind. For example in the *Layered Vertex Cover* problem: given a graph $G = (V, E)$. and parameter (k, k', k'') the question is can we delete k vertices from G, obtaining G' such that every connected component C of G' has the property that: k' vertices can be deleted from C resulting in a graph C'' such that each connected component of C'' has a vertex cover of size at most k''?

Or perhaps our particular application intention might be naturally served by deleting k vertices so that the resulting connected components have nice properties governed by a parameter t, and these components can be further decomposed into connected components with a different nice property governed by t' and so on.

Direction 2. The theme of fairly simple and elemental decompositions based on vertex- and edge-cutsets is important.

Direction 3. Since the size n of the networks (graphs) targeted in this application area is huge, the attention should be focused on *truly linear-time FPT*, that is, processing that is simply of $O(n)$ cost, regardless of any parameterization k that we might want to consider. Polynomial time $O(n^c)$ with no exponential costs associated to the parameter k, is the best kind of FPT. For very large graphs, we need $c = 1$. Slightly more generally, we might consider reasonable FPT processing time-costs of the form $O(n^c + f(k))$, where again the exponent of the polynomial part is $c = 1$, which we will call truly linear time FPT. This is an area of PC structural complexity theory little explored. There is a small amount of relevant recent work by Jianer Chen and coauthors.

FPT Approximation of Vertex Bisubsection

Edge (resp. Vertex) Bisubsection is one the fundamental graph partitioning problems, where given a graph G and an integer k, the goal is to find a set of at most k edges (resp. vertices), say S, such that the vertex set of $G \setminus S$ can be partitioned into two almost equal parts V_1 and V_2, that is $||V_1| - |V_2|| \leq 1$, and there are no edges between a vertex of V_1 and

V_2, that is $E(V_1, V_2) = \emptyset$. In the regime of parameterized complexity, Edge Bisubsection admits a fixed-parameter tractable (FPT) algorithm parameterized by the solution size k. In particular, it admits an algorithm running in time $2^{O(k \log k)} n^{O(1)}$ [18], where n is the number of vertices in the input graph.

Open Problem 1. One can solve Edge Bisubsection, for fixed k, in linear time? Preferably, is there an algorithm solving Edge Bisubsection in $2^{O(k \log k)} n$-time?

Open Problem 2. Does Edge Bisubsection admit an algorithm with running time $2^{O(k)} n^{O(1)}$? Or can one show that there is no algorithm for this problem that runs in time $2^{o(k \log k)} n^{O(1)}$ under reasonable complexity assumptions?

In contrast to Edge Bisubsection, Vertex Bisubsection is known to be W[1]-hard [44], that is it is unlikely that it admits an FPT algorithm parameterized by k. On the kernelization front, Edge Bisubsection cannot admit a polynomial kernel under reasonable complexity assumptions [79]. This leads of interesting questions regarding the fixed-parameter tractability and/or kernelization *with approximations* for these problems. In particular, the following questions remain intriguing.

Open Problem 3. Does Edge Bisubsection admit a polynomial α-lossy kernel, for some $\alpha > 1$? Are there lossy reduction rules that help in solving the problem practically?

Open Problem 4. Does Vertex Bisubsection admit an FPT-approximation algorithm? That is, in time $f(k, \epsilon) n^{O(1)}$, can one find a set of at most $(1 + \epsilon)k$ vertices, say S, such that $V(G \setminus S) = V_1 \uplus V_2$, $||V_1| - |V_2|| \leq 1$ and $E(V_1, V_2) = \emptyset$, or report that there is no such set S of size at most k?

Open Problem 5. In scenarios where Vertex Bisubsection pops up in practical usage, can we identify some structure on the instances? For example, can we say that the graphs in interesting instances belong to some nice graph class, or "is close to" being in a graph class (this could, for example, be formalized using distance to triviality measures), or have some bounded parameter. If such an identification is possible, studying these scenarios theoretically may lead to interesting insights about the problem.

FPT in Decomposition

The first open question here is if Densest k-Subgraph *FPT parameterized by modular-width?* Given a graph G and an integer k, the Densest k-Subgraph problem asks for a subgraph of G with at most k vertices maximizing the number of edges. It is known that this problem is FPT by stronger parameters such as neighborhood diversity and twin cover, yet it is W[1]-hard by weaker clique-width. Modular-width is defined using the standard concept of modular decomposition [23]. Any graph can be produced via a sequence of the following operations:

1. Introduce: Create an isolated vertex.
2. Union $G_1 \oplus G_2$: Create the disjoint union of two graphs G_1 and G_2.
3. Join: Given two graphs G_1 and G_2, create the complete join G_3 of G_1 and G_2. That is, a graph G_3 with vertices $V(G_1) \cup V(G_2)$ and edges $E(G_1) \cup E(G_2) \cup \{(v, w) : v \in G_1, w \in G_2\}$.
4. Substitute: Given a graph G with vertices $v_1, \ldots, v_n$ and given graphs $G_1, \ldots, G_n$, create the *substitution* of $G_1, \ldots, G_n$ in G. The substitution is a graph $\mathcal{G}$ with vertex set $\bigcup_{1 \leq i \leq n} V(G_i)$ and edge set $\bigcup_{1 \leq i \leq n} E(G_i) \cup \{(v, w) : v \in G_i, w \in G_j, (v_i, v_j) \in E(G)\}$. Each graph G_i is substituted for a vertex v_i, and all edges between graphs corresponding to adjacent vertices in G are added.

These operations, taken together in order to construct a graph, form a *parse-tree* of the graph. The width of a graph is the maximum size of the vertex set of G used in operation (O4) to construct the graph. The *modular-width* is the minimum width such that G can be obtained from some sequence of operations (1)-(4). Finding a parse-tree of a given graph, called a *modular decomposition*, can be done in linear-time [75].
The second open question is whether we can develop a framework of approximate modular decomposition applicable to real-world datasets? Unfortunately, most real-world graphs tend to have larger modular-width. It would be beneficial if we can efficiently build non-exact parse trees with much lower width but without losing much information. Possible avenues of exploration include graph editing, a relaxed definition of the parse-tree, and a data-driven approach.

Advancing the Parameterized View on Graph Modification

One of the most explored topics in parameterized complexity are so called *distance to triviality problems* (see, for example, [22, 30]). The intuitive question behind these problems is always "can we make a small change to our input so that it takes on some property?". In terms of graph problems, one can state a meta-problem as follows, where $\mathcal{P}$ is a graph property *Vertex-Deletion-To-*$\mathcal{P}$: given a graph G, an integer k as well as a parameter k, the question is can we delete at most k vertices from G, such that the resulting graph has property $\mathcal{P}$?

For many graph properties for which one can consider this meta-problem, either tractable algorithms or complexity lower bounds are known. On the other hand, in some application areas it could be useful to delete as many vertices as possible, while ensuring that the resulting graph has a certain property. This leads to the *Max-Vertex-Deletion-To-*$\mathcal{P}$ problem: given a graph G, an integer k as well as a parameter k, the question is can we delete *at least* k vertices from G, such that the resulting graph has property $\mathcal{P}$?

While the change to the problem statement is deceptively simple, we have to this date no complexity-theoretic insight into this class of problems. Note that this problem also differs from the widely used kernelization techniques, as in kernelization, we ask for the resulting input size to be bounded by, for example, $f(k)$. As parameterized complexity can be seen as providing a mathematically rigorous framework of preprocessing through the rich methods of kernelization techniques and algorithmics for distance to triviality problems, extending this framework to further variants of preprocessing seems very natural and could provide further complexity-theoretic and algorithmic insights. These techniques could potentially be useful in the area of (hyper)graph decomposition.

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