A parallelisable multi-level banded diffusion scheme for computing balanced partitions with smooth boundaries

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Abstract. Graph partitioning algorithms have yet to be improved, because graph-based local optimization algorithms do not compute smooth and globally-optimal frontiers, while global optimization algorithms are too expensive to be of practical use on large graphs. This paper presents a way to integrate a global optimization, diffusion algorithm in a banded multi-level framework, which dramatically reduces problem size while yielding balanced partitions with smooth boundaries. Since all of these algorithms do parallelize well, high-quality parallel graph partitioners built using these algorithms will have the same quality as state-of-the-art sequential partitioners.

1 Introduction

Graph partitioning is an ubiquitous technique which has applications in many fields of computer science and engineering, such as workload balancing in parallel computing, database storage, VLSI design or bio-informatics. It is mostly used to help solving domain-dependent optimization problems modeled in terms of weighted or unweighted graphs, where finding good solutions amounts to computing, eventually recursively in a divide-and-conquer framework, small vertex or edge cuts that balance evenly the weights of the graph parts.

Many algorithms have been proposed to compute efficient partitions of any graphs, such as graph or evolutionary algorithms, spectral methods, or linear optimization methods. Basically, all of these methods belong to two distinct classes: global methods, which consider all of the graph data, and local optimization heuristics, which try to improve locally a pre-existing partition. Global methods often yield better results, but their costs dramatically increases along with the problem size, which makes them practically impossible to use for graphs comprising several tens million vertices, which are the graphs now being considered in many scientific engineering problems.

The multi-level approach [1, 6, 7] has been a quite successful attempt to combine both approaches. It consists in repeatedly computing a set of increasingly coarser albeit topologically similar versions of the graph to partition, by finding

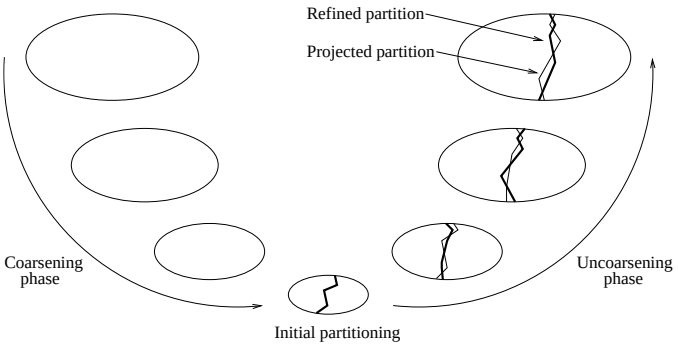

Fig. 1. Multi-level framework for computing a bipartition of a graph.

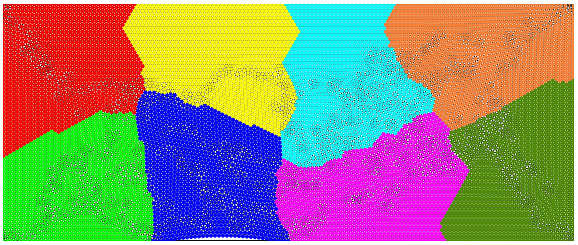

Fig. 2. Partition of graph **bump** into 8 parts with SCOTCH 4.0, using the multi-level framework with the un-banded Fiduccia-Mattheyses refinement algorithm. The cut is equal to 714 edges. Segmented frontiers are clearly evidenced.

matchings which collapse vertices and edges, until the coarsest graph obtained is no larger than a few hundreds of vertices, then computing a separator on this coarsest graph, and projecting back this separator, from coarser to finer graphs, up to the original graph. Most often, a local optimization algorithm, such as Kernighan-Lin [8] or Fiduccia-Mattheyses [5] (FM), is used in the uncoarsening phase to refine the partition that is projected back at every level, such that the granularity of the solution is the one of the original graph and not the one of the coarsest graph, as illustrated in Figure 1. This approach improves quality over plain graph algorithms, and speed over plain global optimization algorithms, by taking the best of both worlds. Global optimization algorithms can be used on small graphs to give the general direction of the partition to set, and unexpensive local optimization algorithms can be used at low cost on finer graphs with tens of million vertices.

However, the quality of partitions yielded by this approach is not as good as the one that would be yielded by plain global optimization algorithms. Coarsening artefacts, as well as the meshing topology of the original graphs, trap local optimization algorithms in local optima of their cost functions, such that frontiers are often made of non-optimal sets of segments, as illustrated in Figure 2.

This paper describes an efficient way to integrate diffusion schemes into a multi-level framework, so as to compute partitions with small and smooth frontiers in a time equivalent in magnitude to the one of state-of-the-art local optimization algorithms.

This paper is organized as follows. After presenting related works in Section 2, we introduce in Section 3 our multi-level banded diffusion scheme, and show some partitioning and mapping results, obtained with SCOTCH 5.0, in Section 4. Then comes the conclusion.

2 Related works

Many authors had already noticed that partitions yielded by local optimization algorithms were not optimal. One of the most vocal communities was the one of the users of iterative linear system solving methods [13], which experienced that such partitions were not fitted for their purpose, as subdomains with longer frontiers or irregular shapes resulted in a larger number of iterations to achieve convergence. To measure the quality of each of the parts, several authors defined a metric called *aspect ratio*, which can be thought in 2D as a measure of the perimeter of a part with respect to the square root of its area. The more compact a part is, the smaller its aspect ratio value is, as ideal parts are of circular shape in the Euclidian space.

In [4], Diekmann *et al.* evidenced such a behavior, and proposed both a measure of the aspect ratio of the parts, as well as a set of heuristics to create and refine the partitions, with the objective of decreasing their aspect ratio. Among these algorithms is a "bubble-growing" algorithm. This algorithm is based on the observation that sets of soap bubbles self-organize so as to minimize the surface of their interfaces, which is indeed what is expected from a partitioning algorithm. Consequently, the authors' idea was to grow, from as many seed vertices as the desired number of parts, a collection of expanding bubbles, by performing breadth-first traversals rooted at these seed vertices. Once every graph vertex has been assigned to some part, each part computes its center based on the graph distance metric. These center vertices are taken as new seeds and the expansion process is started again, until it converges, that is, until centers of subdomains no longer move. An important drawback of this method is that it does not guarantee that all parts will hold the same number of vertices, which requires to call other heuristics in turn to perform load balancing. Also, all of the graph vertices must be visited many times, which makes this algorithm quite expensive, all the more it is combined with costly algorithms such as simulated annealing, and the computation of the aspect ratio requires some knowledge on the geometry of the graphs, which is not always available.

In [9], Meyerhenke and Schamberger further explores the bubble model, and devises a way to grow the bubbles by solving, possibly in parallel, systems of linear equations, instead of iteratively computing bubble centers. This method yields partitions of high quality too, but is very slow, even in parallel [10], and

the load balancing problem is also not addressed, which requires to resort to a greedy load balancing algorithm afterwards.

In [14], Wan *et al.* explore a diffusive model, called the *influence model*, where vertices impact their neighbors by diffusing them information on their current state. This model also does not handle load balancing properly.

3 Multi-level banded diffusion scheme

In spite of their better quality, all of the above diffusion schemes have two drawbacks: first, they do not naturally balance loads between parts and second, they are expensive as they involve all of the graph vertices. The method that we propose here addresses both of these problems.

3.1 The jug of the Danaides

The diffusion scheme that we propose can apply to an arbitrary number of parts, but for the sake of clarity we will describe it in the context of graph bipartitioning, that is, with two parts only. We model the graph to bipartition in the following way, depicted in Figure 3. Nodes are represented as barrels of infinite capacity, which leak such that one unit of liquid at most drips per unit of time. When graph vertices are weighted, always with integer weights, the maximum quantity of liquid to be lost per unit of time is equal to the weight of the vertex. Graph edges are modeled by pipes of section equal to their weight. In both parts, a source vertex is chosen, to which a source pipe is connected, which flows in $\frac{|V|}{2}$ units of liquid per unit of time. Two sorts of liquids are in fact injected in the system: water in the first pipe, and anti-water in the second pipe, such that when some quantity of water mixes with the same quantity of anti-water, both vanish. To ease the writing of the algorithm in the bipartitioning case, water is represented by positive quantities and anti-water is represented by negative ones, so that mutual destruction naturally takes place when adding any two quantities of opposite signs.

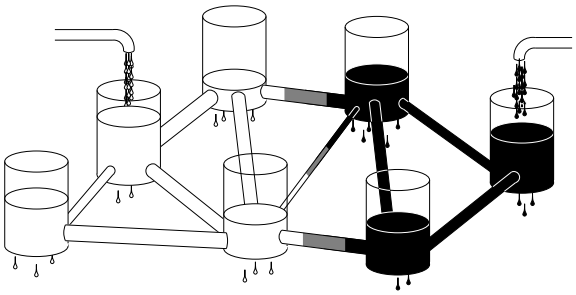

Fig. 3. Sketch of our diffusion model.

The diffusion algorithm performs as outlined in Figure 4. For each time step, and for each vertex, the amount of liquid (whether water or anti-water) which remains after some has leaked is spread across the connecting pipes towards the neighboring barrels, according to their relative sections. This process could be iterated until convergence, but in fact is only performed for a number of steps sufficient to achieve sign stability. Indeed, we are not interested in complete convergence, but in the stability of the signs of all content quantities beared by the graph vertices, which indicate whether water or anti-water dominates in the barrels, that is, if some vertex belongs to part 0 or 1.

Since $|V|$ units of both liquids are injected on the whole per unit of time, and since all of the barrels can leak the same overall amount in the same time, the system is bound to converge, all the more that liquid can disappear by collision of water and anti-water. As in the bubble schemes, what is expected is that a smooth front will be created between the two parts. The purpose of the algorithm is more to have a global smoothing of the frontier than a strict minimization of the cut. In fact, unlike all of the algorithms presented in the previous section, our method privileges load balancing over cut minimization. For this latter criterion, we rely on an additional feature of our scheme, as explained below.

3.2 Band graphs in a multi-level scheme

Our diffusion algorithm, as such, presents two weaknesses: nothing is said about the selection of the seed vertices, and performing such iterations over all of the graphs vertices is very expensive compared to local optimization algorithms which only consider vertices in the immediate vicinity of the frontiers.

To address these two problems concurrently, we use a method we have developed in [2], illustrated in Figure 5. It consists in using a multi-level scheme in which refinement algorithms are not applied to the full graphs but to band graphs that contain vertices that are at most at some small distance, typically 3, from the projected separator. In these band graphs, two additional "anchor" vertices represent all of the removed vertices of each part, and are connected to the last band layers of vertices of each of the parts. The vertex weight of the anchor vertices is equal to the sum of the vertex weights of all of the vertices they replace, to preserve the balance of the two band parts.

The underlying reasoning of this pre-constrained banding scheme is that since every refinement is classically performed by means of a local algorithm, which perturbs only in a limited way the position of the projected separator, local refinement algorithms need only to be passed a subgraph that contains the vertices that are very close to the projected separator. We have experimented that, when performing Fiduccia-Mattheyses refinement on band graphs that contain only vertices that are at distance at most 3 from the projected separators, the quality of the finest separator does not only remain constant, but even significantly improves in most cases. Our interpretation is that this pre-constrained banding prevents the local optimization algorithms from exploring and being trapped in local optima that would be too far from the global optimum sketched at the coarsest level of the multi-level process.

```
while (number of passes to do) {
  reset contents of new array to 0;
  old[s0] ← old[s0] − |V|/2;          /* Refill source barrels */
  old[s1] ← old[s1] + |V|/2;
  for (all vertices v in graph) {
    c ← old[v];                       /* Get contents of barrel            */
    if (|c| > weight[v]) {            /* If not all contents have leaked   */
      c ← c − weight[v] ∗ sign(c);    /* Compute what will remain          */
      σ ← Σ_{e=(v,v')} weight[e];     /* Sum weights of all adjacent edges */
      for (all edges e = (v, v')) {   /* For all edges adjacent to v       */
        f ← c ∗ weight[e]/σ;          /* Fraction to be spread to v'       */
        new[v'] ← new[v'] + f;        /* Accumulate spreaded contributions */
      }
    }
  }
  swap old and new arrays;
}
```

Fig. 4. Sketch of the jug-of-the-Danaides diffusion algorithm. Water, represented as positive quantities, flows from the source of part 1, while anti-water, represented as negative quantities, flows from the source of part 0. For each step, the current and new contents of every vertex are stored in arrays `old` and `new`, respectively.

Such a banded scheme is ideal for using our diffusion scheme, as anchor vertices represent a natural choice to be taken as seed vertices. Indeed, the most important problem for bubble-growing algorithms is the determination of the seed vertices from which bubbles are grown, which requires expensive processes involving all of the graph vertices [4, 9]. Since anchor vertices are connected to all of the vertices of the last layers, the diffused liquids flow as a front as if they originated from the farthest vertices from the frontier, which is indeed what would happen if they flowed from the center of a bubble having the frontier as its perimeter.

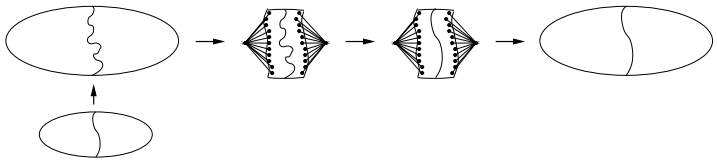

Fig. 5. Multi-level banded refinement scheme. A band graph of small width is created around the projected finer separator, with anchor vertices representing all of the removed vertices in each part. After some optimization algorithm (whether local or global) is applied, the refined band separator is projected back to the full graph, and the uncoarsening process goes on.

Graph	Size ($\times 10^3$)		Average degree
	$\|V\|$	$\|E\|$	
altr4	26	163	12.50
bmw32	227	5531	48.65

Table 1. Description of some of the test graphs that we use. $|V|$ and $|E|$ are the vertex and edge cardinalities, in thousands.

3.3 Parallelization

Our diffusion algorithm has the additional interest of being highly scalable. If we assume that full graphs, as well as band graphs, are distributed across processors such that every processor holds a fraction of the graph vertices along with their adjacency lists, like what is done for instance in PT-Scotch [3], the parallel version of Scotch, the parallel version of the algorithm is straightforward. Every processor performs its local update and computes the contributions it has to spread to distant neighbors, after which these contributions are sent to their destination processors in order to be aggregated. In order to cover communication by computations, vertices that have distant neighbors can be processed first, then communications are started, and vertices with purely local adjacency lists can be processed in the mean time, before received contributions are aggregated.

4 Experimental results

The diffusion algorithm discussed above has been implemented, as a sequential graph bipartitioning method, in the Scotch [11] graph partitioning and static mapping software, and will be released in the upcoming version 5.0. Its k-way implementation is not yet available, because it requires more coding, including a k-way band extraction algorithm which does not exist to date. All of the necessary floating-point arithmetics have been implemented in single-precision.

The tests were run on a Lenovo ThinkPad T60 laptop, with an Intel dual-core T2400 processor running at 1.8 MHz and 1 Gb of memory. As we ran sequential tests only, the dual-core feature of the processor is not relevant. Some of the test graphs we have used in our experiments are listed in Table 1. These graphs were partitioned into 2 to 128 parts, and the two quality metrics that we consider are the number of cut edges, called **Cut**, and the maximum diameter of the parts, referred to as **MDi**, which is an indirect metric of the shape of the partition, and which is also relevant in the case of graphs of unknown or unexisting geometry. The best proof would have been to run an iterative solver and compare convergence rates basing on the numbers of iterations, but this could not be done by lack of time.

Three heuristics were compared. The first one is the classical strategy implemented in Scotch `4.0`, that is, recursive bipartitioning with bipartitions computed in a multi-level way, using FM refinement; it is referred to as MF.

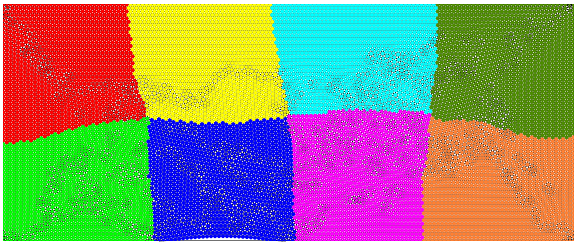

Fig. 6. Partition of graph **bump** into 8 parts with SCOTCH 5.0, using the MBDF strategy. The cut is equal to 713 edges.

The second one, MBD, uses the same strategy, but banded diffusion is performed during the refinement steps. This strategy has been evaluated, but its results are disappointing, resulting in too much load imbalance between parts; therefore, it is not included in our results. The third one, MBDF, also uses band graphs during the refinement process, and calls the diffusion algorithm on the band graph, but afterwards also calls the FM algorithm on the resulting band partition. The idea of this strategy is to benefit from the global optimization capabilities brought by the diffusion algorithm, while locally optimizing the frontier afterwards. Finally, as a comparison, results obtained with K-METIS are also included in our tables. K-METIS uses direct k-way partitioning instead of recursive bipartitioning, which usually makes it more efficient when the number of parts increases, and also much faster (from 10 to 20 times). Timings are not included to save space, but it has been consistently found that the time taken by MBDF is four times the one taken by MF, when performing 40 diffusion steps per run.

Some partitioning results are given as examples in Table 2, and represent the general trend. The MBDF strategy results in an increase of the cut size by about 5 percent on average compared to MF, but by a decrease of the maximum diameters of the parts. Both phenomena can be experienced in Figure 6, to be compared with Figure 2; parts are visually more compact, but straight diffusion frontiers may not fully take advantage of the topology to reduce the cut. The same smoothing of frontiers is also visible for complex 3D graphs.

As analyzed in [12], the performance of recursive bipartitioning methods tends to decrease when the number of parts increases, which limits the efficiency of the MBDF method for large number of parts. A full k-way algorithm is required.

5 Conclusion and future work

In this paper, we have presented a diffusion algorithm which, used in a multi-level banded framework, results in smoother partition frontiers and more compact parts. Used in this banded context, this algorithm is fast enough to be used on very large graphs, as it is only four times slower than classical local optimization

Test case		Number of parts						
		2	4	8	16	32	64	128
altr4								
MF	**Cut**	1688	**3197**	**4978**	**7788**	**11905**	17656	24478
	MDi	50	52	40	**33**	**25**	21	**14**
MBDF	**Cut**	**1624**	3408	5151	8043	12268	17825	25623
	MDi	**48**	**48**	**38**	34	**25**	**19**	16
KMeT	**Cut**	1670	3233	4981	8115	12147	**17355**	**24058**
	MDi	**48**	45	41	34	26	22	**14**
bmw32								
MF	**Cut**	17271	**54424**	84222	**120828**	**181844**	**267427**	**394418**
	MDi	93	116	130	106	74	120	**68**
MBDF	**Cut**	**14922**	62956	**76369**	123618	188657	285139	422992
	MDi	92	**104**	**92**	**86**	**68**	70	115
KMeT	**Cut**	15529	55506	92658	125686	193169	286111	420965
	MDi	**87**	108	99	87	70	**61**	**68**

Table 2. Comparison of the results, in terms of cut size (**Cut**) and maximum diameter of the parts (**MDi**), between four heuristics: multi-level with FM refinement (MF, as implemented in Scotch 4.0), multi-level with banded diffusion plus banded FM refinements (MBDF), and K-MeTiS (KMeT).

schemes. The 2-way sequential version has been integrated in version 5.0 of Scotch, to be released soon.

This algorithm is also easily parallelizable and highly scalable, which makes it a very good candidate for the realization of a fast and efficient parallel graph partitioner, taking advantage of the parallel multi-level and band graph extraction routines already developed in PT-Scotch in the context of sparse matrix reordering [3].

A k-way version of the algorithm is under development, which extends the 2-way model by considering k different liquids with the same annihilation properties, such that when p different liquids are mixed in the same barrel, only the most abundant one remains. This behavior is equivalent to the one of our algorithm in the 2-way case. Using a native k-way scheme should also significantly reduce running times compared to recursive bipartitioning.

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