Multilevel Mesh Partitioning for Optimising Subdomain Aspect Ratio

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Abstract

Multilevel algorithms are a successful class of optimisation techniques which address the mesh partitioning problem for mapping meshes onto parallel computers. They usually combine a graph contraction algorithm together with a local optimisation method which refines the partition at each graph level. To date these algorithms have been used almost exclusively to minimise the cut-edge weight in the graph with the aim of minimising the parallel communication overhead. However it has been shown that for certain classes of problem, the convergence of the underlying solution algorithm is strongly influenced by the shape or aspect ratio of the subdomains. In this paper therefore, we modify the multilevel algorithms in order to optimise a cost function based on aspect ratio. Several variants of the algorithms are tested and shown to provide excellent results.

1 Introduction

The need for mesh partitioning arises naturally in many finite element (FE) and finite volume (FV) applications. Meshes composed of elements such as triangles or tetrahedra are often better suited than regularly structured grids for representing completely general geometries and resolving wide variations in behaviour via variable mesh densities. Meanwhile, the modelling of complex behaviour patterns means that the problems are often too large to fit onto serial computers, either because of memory limitations or computational demands, or both. Distributing the mesh across a parallel computer so that the computational load is evenly balanced and the data locality maximised is known as mesh partitioning. It is well known that this problem is NP-complete, so in recent years much attention has been focused on developing suitable heuristics, and some powerful methods, many based on a graph corresponding to the communication requirements of the mesh, have been devised, e.g. [15].

A particularly popular and successful class of algorithms which address this mesh partitioning problem are known as multilevel algorithms. They usually combine a graph contraction algorithm which creates a series of progressively smaller and coarser graphs together with a local optimisation method which, starting with the coarsest graph, refines the partition at each graph level. To date these algorithms have been used almost exclusively to minimise the cut-edge weight, a cost which approximates the total communications volume in the underlying solver. This is an important goal in any parallel application, in order to minimise the communications overhead, however, it has been shown, [24], that for certain classes of solution algorithm, the convergence of the solver is actually heavily influenced by the shape or aspect ratio (AR) of the subdomains and in this case the overall solution time can be more dependent on the number of iterations than on the parallel communications overhead, [23]. In this paper therefore, we modify the multilevel algorithms (the matching and local optimisation) in order to optimise a cost function based on AR. We also abstract the process of modification in order to suggest how the multilevel strategy can be modified into a generic technique which can optimise arbitrary cost functions.

1.1 Domain decomposition preconditioners and aspect ratio

To motivate the need for aspect ratio optimisation we consider the requirements of a class of solution techniques. A natural *parallel* solution strategy for the underlying problem is to use an iterative solver such as the conjugate gradient (CG) algorithm together with domain decomposition (DD) preconditioning, e.g. [3]. DD methods take advantage of the partition of the mesh into subdomains by imposing artificial boundary conditions on the subdomain boundaries and solving the original problem on these subdomains, [5]. The subdomain solutions are independent of each other, and thus can be determined in parallel without any communication between processors. In a second step, an 'interface' problem is solved on the inner boundaries which depends on the jump of the subdomain solutions over the boundaries. This interface problem gives new conditions on the inner boundaries for the next step of subdomain solution. Adding the results of the third step to the first gives the new conjugate search direction in the CG algorithm.

The time needed by such a preconditioned CG solver is determined by two factors, the maximum time needed by any of the subdomain solutions and the number of iterations of the global CG. Both are at least partially determined by the shape

of the subdomains. Whilst an algorithm such as the multigrid method as the solver on the subdomains is relatively robust against shape, the number of global iterations are heavily influenced by the AR of subdomains, [23]. Essentially, the subdomains can be viewed as elements of the interface problem, [10, 11], and just as with the normal finite element method, where the condition of the matrix system is determined by the AR of elements, the condition of the preconditioning matrix is here dependent on the AR of subdomains.

1.2 Related work

The idea of optimising AR in order to maintain scalability in the solver was first developed by Farhat *et al.*, [10, 11]. This was backed up by Vanderstraeten *et al.* who showed that partitioning for cut-edge weight was not necessarily the most appropriate optimisation for every solver [23, 24]. However the field of mesh partitioning has changed somewhat since this work was carried out and although other more recent work exists which takes AR into account, e.g. [7, 8, 22], our aim in this paper is to extend the ideas in the light of recent developments in multilevel mesh partitioning technology.

1.3 Overview

Below, in Section 2, we introduce the mesh partitioning problem and establish some terminology. We then discuss the mesh partitioning problem as applied to AR optimisation and describe how the graph needs to be modified to carry this out. Next, in Section 3, we describe the multilevel paradigm and present and compare three possible matching algorithms which take account of AR. In Section 4 we then outline a Kernighan-Lin (KL), [18], type iterative local optimisation algorithm and describe four possible modifications which aim to optimise AR. Finally in Section 5 we compare the results with a cut edge partitioner, suggest how the multilevel strategy can be modified into a generic technique and present some ideas for further investigation.

2 Mesh partitioning

2.1 The mesh partitioning problem

To define the mesh partitioning problem, let $G = G(V, E)$ be an undirected graph of vertices V, with edges E which represent the data dependencies in the mesh. For the purposes of this paper we assume that each graph vertex represents a mesh element and that graph edges arise from elements that are adjacent in the sense of sharing an element face. We assume that both vertices and edges can be weighted (with positive integer values) and that $|v|$ denotes the weight of a vertex v and similarly for edges and sets of vertices and edges. Given that the mesh needs to be distributed to P processors, define a partition π to be a mapping of V into P disjoint subdomains S_p such that $\bigcup_P S_p = V$. To evenly balance the load, the optimal subdomain weight is given by $\overline{S} := \lceil |V|/P \rceil$ (where the ceiling function $\lceil x \rceil$ returns the smallest integer $\geq x$) and the *imbalance* is then defined as the maximum subdomain weight divided by the optimal (since the computational speed of the underlying application is determined by the most heavily weighted processor).

The definition of the mesh-partitioning problem then is to find a partition which evenly balances the load or vertex weight in each subdomain whilst minimising some cost function Γ. Typically this cost function is simply the total weight of cut edges, but in this paper we describe a cost function based on AR. A more precise definition of the mesh-partitioning problem is therefore to find π such that $S_p \leq \overline{S}$ and such that Γ is minimised.

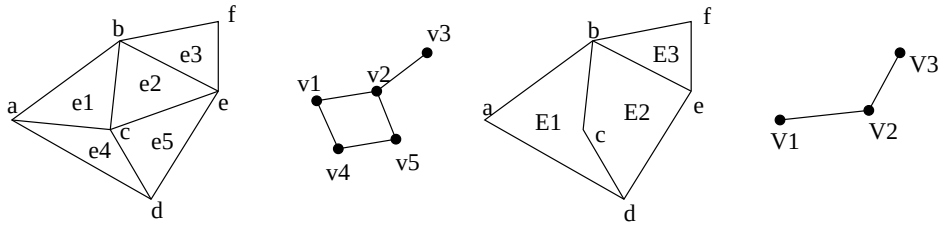
2.2 The aspect ratio and cost function

We seek to modify the methods by optimising the partition on the basis of AR rather than cut-edge weight. In order to do this it is necessary to define a cost function which we seek to minimise and a logical choice would be $\max_p \mathrm{AR}(S_p)$, where $\mathrm{AR}(S_p)$ is the AR of the subdomain S_p. However maximum functions are notoriously difficult to optimise (indeed it is for this reason that most mesh partitioning algorithms attempt to minimise the total cut-edge weight rather than the maximum between any two subdomains) and so instead we choose to minimise the average AR

$$\Gamma_{\text{AR}} = \sum_p \frac{\mathrm{AR}(S_p)}{P}. \tag{1}$$

There are several definitions of AR, however, and for example, for a given polygon S, a typical definition, [21], is the ratio of the largest circle which can be contained entirely within S (inscribed circle) to the smallest circle which entirely contains S (circumcircle). However these circles are not easy to calculate for arbitrary polygons and in an optimisation code where ARs may need to be calculated very frequently, we do not believe this to be a practical metric. It may also fail to express certain irregularities of shape. A careful discussion of the relative merits of different ways of measuring AR may be found in [22] and for the purposes of this paper we follow the ideas therein and define the AR of a given shape by measuring the ratio of its perimeter length (surface area in 3d) over that of some ideal shape with identical area (volume in 3d).

Suppose then that in 2d the ideal shape is chosen to be a square. Given a polygon S with area ΩS and perimeter length ∂S, the ideal perimeter length (the perimeter length of a square with area ΩS) is $4\sqrt{\Omega S}$ and so the AR is defined as $\partial S / 4\sqrt{\Omega S}$. Alternatively, if the ideal shape is chosen to be a circle then the same argument gives the AR of $\partial S / 2\sqrt{\pi \Omega S}$. In fact, given the definition of the cost function (1) it can be seen that these two definitions will produce the same optimisation problem (and hence the same results) with the cost just modified by a constant C (where $C = 1/4$ for the square and $1/2\sqrt{\pi}$ for circle). These definitions of AR are easily extendible to 3d and given a polyhedron S with volume ΩS and surface area ∂S, the AR can be calculated as $C \partial S / (\Omega S)^{2/3}$, where $C = 1/4$ if



(a) (b) (c) (d)

Figure 1: Left to right: a simple mesh (a), its dual (b), the same mesh with combined elements (c) and its dual (d)

the cube is chosen as the optimal shape and $C = 1/\pi^{1/3}6^{2/3}$ for the sphere. Note that henceforth, in order to talk in general terms for both 2d & 3d, given an object S we shall use the terms ∂S or *surface* for the surface area (3d) or perimeter length (2d) of the object and ΩS or *volume* for the volume (3d) or area (2d).

Of the above definitions of AR we choose to use the circle/sphere based formulae since they guarantee that the aspect ratios of any shape are ≥ 1. This gives a convenient formula for the cost function of:

$$\Gamma_{\text{template}} = \frac{1}{C} \sum_p \frac{\partial S_p}{(\Omega S_p)^{\frac{d-1}{d}}} \tag{2}$$

where $C = \pi^{\frac{1}{d}}(2d)^{\frac{d-1}{d}}P$ and d (= 2 or 3) is the dimension of the mesh. We refer to this cost function as Γ_{template} or Γ_t because of the way it tries to match shapes to chosen templates.

In fact, it will turn out (see for example §3.2) that even this function may be too complex for certain optimisation needs and we can define a simpler one by assuming that all subdomains have approximately the same volume, $\Omega S_p \approx \Omega M/P$, where ΩM is the total volume of the mesh. This assumption may not necessarily be true, but it is likely to be true locally (see §4.4). We can then approximate (2) by

$$\Gamma_{\text{template}} \approx \frac{1}{C'} \sum_p \partial S_p \tag{3}$$

where $C' = (\pi P)^{\frac{1}{d}}(2d\Omega M)^{\frac{d-1}{d}}$. This can be simplified still further by noting that the surface of each subdomain S_p consists of two components, the *exterior* surface, $\partial^e S_p$, where the surface of the subdomain coincides with the surface of the mesh ∂M, and the *interior* surface, $\partial^i S_p$, where S_p is adjacent to other subdomains and the surface cuts through the mesh. Thus we can break the $\sum_p \partial S_p$ term in (3) into two parts $\sum_p \partial^i S_p$ and $\sum_p \partial^e S_p$ and simplify (3) further by noting that $\sum_p \partial^e S_p$ is just ∂M, the exterior surface of the mesh M. This then gives us a second cost function to optimise:

$$\Gamma_{\text{surface}} = \frac{1}{K_1} \sum_p \partial^i S_p + K_2 \tag{4}$$

where $K_1 = (\pi P)^{\frac{1}{d}}(2d\Omega M)^{\frac{d-1}{d}}$ and $K_2 = \partial M/K_1$. We refer to this cost function as Γ_{surface} or Γ_s because it is just concerned with optimising surfaces.

2.3 Modifying the graph

To use these cost functions in a graph-partitioning context, we must add some additional qualities to the graph. Figure 1 shows a very simple mesh (1a) and its dual graph (1b). Each element of the mesh corresponds to a vertex in the graph. The vertices of the graph can be weighted as is usual (see §2.1) but in addition, vertices store the volume and total surface of their corresponding element (e.g. $\Omega v_1 = \Omega e_1$ and $\partial v_1 = \partial e_1$). We also weight the edges of the graph with the size of the surface they correspond to. Thus, in Figure 1, if $D(b, c)$ refers to the distance between points b and c, then the weight of edge (v_1, v_2) is set to $D(b, c)$. In this way, for vertices v_i corresponding to elements which have no exterior surface, the sum of their edge weights is equivalent to their surface ($\partial v_i = \sum_E |(v_i, v_j)|$). Thus for vertex v_2, $\partial v_2 = \partial e_2 = D(b, c) + D(c, e) + D(e, b) = |(v_2, v_1)| + |(v_2, v_5)| + |(v_2, v_3)|$.

When it comes to combining elements together, either into subdomains, or for the multilevel matching (§3) these properties, volume and surface can be easily combined. Thus in Figure 1(c) where $E_1 = e_1 + e_4$, $E_2 = e_3 + e_5$ and $E_3 = e_3$ we see that volumes can be directly summed, for example $\Omega V_1 = \Omega E_1 = \Omega e_1 + \Omega e_4 = \Omega v_1 + \Omega v_4$, as can edge weights, e.g. $|(V_1, V_2)| = D(b, c) + D(c, d) = |(v_1, v_2)| + |(v_4, v_5)|$. The surface of a combined object S is the sum of the surfaces of its constituent parts less twice the interior surface, e.g. $\partial V_1 = \partial E_1 = \partial e_1 + \partial e_4 - 2 \times D(a, c) = \partial v_1 + \partial v_4 - 2|(v_1, v_4)|$. These properties are very similar to properties in conventional graph algorithms, where the volume combines in the same way as weight and surfaces combine as the sum of edge weights (although including an additional term which expresses the exterior surface ∂^e). The edge weights function identically.

Note that with these modifications to the graph, it can be seen that if we optimise using the Γ_s cost function (4), the AR mesh partitioning problem is identical to the cut-edge weight mesh partitioning problem with a special edge weighting. However, the inclusion of non-integer edge weights does have an effect on the some of the techniques that can be used, in particular the bucket sorting strategy and this is discussed in [27].

2.4 Testing the algorithms

Throughout this paper we compare the effectiveness of different approaches using a set of test meshes. The algorithms have been implemented within the framework of JOSTLE,

mesh	no. vertices	no. edges	type	aspect ratio	mesh grading
uk	4824	6837	2d triangles	3.82	7.98e+02
4elt-dual	30269	44929	2d triangles	1.08	2.13e+04
t60k	60005	89440	2d triangles	1.80	2.00e+00
dime20	224843	336024	2d triangles	2.11	3.70e+03
cs4	22499	43858	3d tetrahedra	1.32	9.64e+01
wing	62032	121544	3d tetrahedra	1.27	1.08e+06
mesh100	103081	200976	3d tetrahedra	2.02	2.45e+02
cyl3	232362	457853	3d tetrahedra	1.59	8.42e+00

Table 1: Test meshes

a mesh partitioning software tool developed at the University of Greenwich and freely available for academic and research purposes under a licensing agreement (available from `http://www.gre.ac.uk/jostle`). The experiments were carried out on a DEC Alpha with a 466 MHz CPU and 1 Gbyte of memory. Due to space considerations we only include 8 test meshes but they have been chosen to be a representative sample of medium to large scale real-life problems and include both 2d and 3d examples. Table 1 gives a list of the meshes and their sizes in terms of the number of vertices and edges. The table also shows the aspect ratio of each entire mesh and the mesh grading, which here we define as the maximum surface of any element over the minimum surface, and these two figures give a guide as to how difficult the optimisation may be. For example, 'uk' is simply a triangulation of the British mainland and hence has a very intricate boundary and therefore a high aspect ratio. The 'wing' mesh on the other hand is a cube containing a hollowed out section in the shape of an aeroplane wing; the AR is therefore reasonably close to 1, but the grading is very high as the mesh goes from very small elements close to the wing to very large ones in the far-field.

Table 2 shows the results of the most successful combination of algorithms – surface matching (SM, see §3.2) and local template gain/template cost optimisation (LTGTC, see §4.3) – which were chosen as a benchmark for the other combinations. For the 4 different values of P (the number of subdomains), the table shows the average aspect ratio as given by Γ_t, the edge cut $|E_c|$ (that is the number of cut edges, not the weight of cut edges weighted by surface size) and the time in seconds, t_s, to partition the mesh. Notice that with the exception of the 'uk' mesh and $P = 16$, all partitions have average aspect ratios ≤ 1.53 which is within the target range of $[1.0, 1.57]$ suggested in [8][1]. Indeed for the 'uk' mesh it is no surprise that the results for $P = 16$ are not optimal because the subdomains inherit some of the poor AR from the original mesh (which has an AR of 3.82) and it is only when the mesh is split into small enough pieces, $P = 32$, 64 or 128, that the optimisation succeeds in ameliorating this effect. Intuitively this also gives a hint as to why DD methods are a very successful technique as a solver.

The partitioning times ranged from under 1 second to a maximum of 16 seconds (for the largest 3D mesh). Experience suggests that this is not an unreasonable overhead for a domain decomposition based method.

3 The multilevel paradigm

In recent years it has been recognised that an effective way of both speeding up partition refinement and, perhaps more importantly giving it a global perspective is to use multilevel techniques. The idea is to match pairs of vertices to form *clusters*, use the clusters to define a new graph and recursively iterate this procedure until the graph size falls below some threshold. The coarsest graph is then partitioned and the partition is successively optimised on all the graphs starting with the coarsest and ending with the original. This sequence of contraction followed by repeated expansion/optimisation loops is known as the multilevel paradigm and has been successfully developed as a strategy for enhancing many partitioning approaches. The multilevel idea was first proposed by Barnard & Simon, [2], as a method of speeding up spectral bisection. It was subsequently generalised by Hendrickson & Leland, [14], who employed it to give global partition quality to local refinement algorithms such as that of Kernighan & Lin [18] and by Vanderstraeten *et al.*, [23], who used it to speed up stochastic optimisation techniques such as simulated annealing, [19]. Several algorithms for carrying out the matching have been devised by Karypis & Kumar, [16], while Walshaw & Cross describe a method for utilising imbalance in the coarsest graphs to enhance the final partition quality, [25].

3.1 Implementation

Graph contraction. To create a coarser graph $G_{l+1}(V_{l+1}, E_{l+1})$ from $G_l(V_l, E_l)$ we use a variant of the edge contraction algorithm proposed by Hendrickson & Leland, [14]. The idea is to find a maximal independent subset of graph edges, or a *matching* of vertices, and then collapse them. The set is independent because no two edges in the set are incident on the same vertex (so no two edges in the set are adjacent), and maximal because no more edges can be added to the set without breaking the independence criterion. Having found such a set, each selected edge is collapsed and the vertices, $u_1, u_2 \in V_l$ say, at either end of it are merged to form a new vertex $v \in V_{l+1}$ with weight $|v| = |u_1| + |u_2|$.

The initial partition. Having constructed the series of graphs until the number of vertices in the coarsest graph is smaller than some threshold, the normal practice of the multilevel strategy is to carry out an initial partition. Here, following the

[1] Reference [8] suggests value of 1.40 using the square/cube based definition of AR in §2.2 – this is equivalent to 1.57 using the circle/sphere based definition.

	$P=16$			$P=32$			$P=64$			$P=128$		
mesh	Γ_t	$\|E_c\|$	t_s	Γ_t	$\|E_c\|$	t_s	Γ_t	$\|E_c\|$	t_s	Γ_t	$\|E_c\|$	t_s
uk	1.62	197	0.27	1.46	332	0.40	1.40	559	0.48	1.40	937	1.08
4elt-dual	1.24	898	0.88	1.28	1358	1.18	1.27	1985	1.40	1.29	2737	1.82
t60k	1.34	1031	1.37	1.28	1607	1.62	1.30	2524	2.03	1.31	3806	2.80
dime20	1.43	1889	4.92	1.34	2886	5.32	1.30	4651	6.15	1.26	6732	7.17
cs4	1.47	2625	2.00	1.47	3660	2.52	1.47	5000	3.23	1.48	6629	3.57
wing	1.37	9346	4.67	1.40	13640	6.48	1.41	15706	7.57	1.43	17027	10.27
mesh100	1.53	6020	4.23	1.49	8413	7.23	1.49	11577	6.38	1.50	15995	8.00
cyl3	1.47	10929	8.68	1.52	16382	10.05	1.52	22355	12.03	1.51	29926	15.97

Table 2: Final results using surface matching and local template gain/template cost optimisation

(a) surface matching (b) cost matching

Figure 2: Surface (a) and cost (b) matching

idea of Gupta, [13], we contract until the number of vertices in the coarsest graph is the same as the number of subdomains, P, and then simply assign vertex i to subdomain S_i. Unlike Gupta, however, we do not carry out repeated expansion/contraction cycles of the coarsest graphs to find a well balanced initial partition but instead, since our optimisation algorithm incorporates balancing (of the vertex weights – see §2.1), we commence on the expansion/optimisation sequence immediately.

Partition expansion. Having optimised the partition on a graph G_l, the partition must be interpolated onto its parent G_{l-1}. The interpolation itself is a trivial matter; if a vertex $v \in V_l$ is in subdomain S_p then the matched pair of vertices that it represents, $v_1, v_2 \in V_{l-1}$, will be in S_p.

3.2 Incorporating aspect ratio

The matching part of the multilevel strategy can be easily modified in several ways to take AR into account and in each case the vertices are visited (at most once) using a randomly ordered linked list. Each vertex is then matched with an unmatched neighbour using the chosen matching algorithm and it and its match removed from the list. Vertices with no unmatched neighbours remain unmatched and are also removed. In addition to **Random Matching (RM)**, [15], where vertices are matched with random neighbours, we propose and have tested 3 matching algorithms:

Surface Matching (SM). As we have seen in §2.3, the AR partitioning problem can be approximated by the cut-edge weight problem using (4), the Γ_s cost function, and so the simplest matching is to use the Heavy Edge approach of Karypis & Kumar, [16], where the vertex matches across the heaviest edge to any of its unmatched neighbours. This is the same as matching across the largest surface (since here edge weights represent surfaces) and we refer to this as *surface matching*.

Template Cost Matching (TCM). A second approach follows the ideas of Bouhmala, [4], and matches vertices with the neighbour which minimises the given cost function. In this case, the chosen vertex matches with the unmatched neighbour which gives the resulting cluster the best aspect ratio. Using the Γ_t cost function, we refer to this as *template cost matching*.

Surface Cost Matching (SCM). This is the same idea as TCM only using the Γ_s cost function, (4), which is faster to calculate and matches a vertex with the neighbour which minimises the surface of the resulting cluster.

Figure 2 motivates the difference between surface matching (SM) and cost matching (SCM & TCM). For surface matching, the graph vertex corresponding to e_1 matches across the largest surface area, in this case with e_2. For cost matching, the graph vertex corresponding to e_1 matches to minimise aspect ratio (TCM) or surface area (SCM) of the resulting cluster, in this case with e_3.

3.3 Results for different matching functions

In Table 3 we compare the results in Table 2, where SM was used, with random matching, RM. In both cases the LTGTC optimisation algorithm (see §4.3) was used. For each value of P, the first column shows the average AR, Γ_t of the partitioning. The second column for each value of P then compares results with those in Table 2 using the metric $\frac{\Gamma(\text{RM})-1}{\Gamma(\text{SM})-1}$. Thus a figure > 1 means that RM has produced worse results than SM.

	$P=16$		$P=32$		$P=64$		$P=128$	
mesh	Γ_t	$\frac{\Gamma(\text{RM})-1}{\Gamma(\text{SM})-1}$	Γ_t	$\frac{\Gamma(\text{RM})-1}{\Gamma(\text{SM})-1}$	Γ_t	$\frac{\Gamma(\text{RM})-1}{\Gamma(\text{SM})-1}$	Γ_t	$\frac{\Gamma(\text{RM})-1}{\Gamma(\text{SM})-1}$
uk	1.65	1.05	1.49	1.06	1.40	1.01	1.39	0.98
4elt-dual	1.29	1.20	1.30	1.09	1.29	1.05	1.29	1.02
t60k	1.36	1.08	1.36	1.26	1.36	1.19	1.37	1.20
dime20	1.45	1.05	1.39	1.16	1.39	1.29	1.35	1.33
cs4	1.58	1.24	1.52	1.12	1.55	1.17	1.53	1.10
wing	1.44	1.17	1.44	1.12	1.44	1.08	1.46	1.07
mesh100	1.59	1.10	1.52	1.05	1.53	1.08	1.57	1.13
cyl3	1.53	1.11	1.52	1.00	1.59	1.14	1.56	1.10
Average		1.12		1.11		1.13		1.12

Table 3: Random matching results compared with surface matching

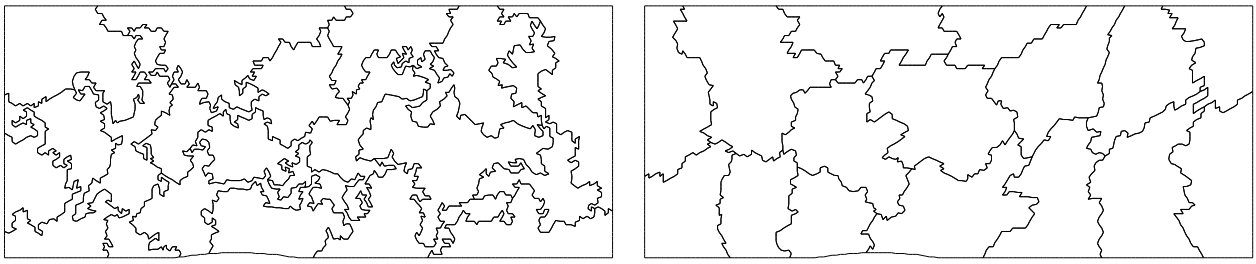


Figure 3: Final 'element' shapes for random (a) and surface (b) matching

These comparisons are then averaged and so it can be seen, e.g. for $P = 16$ that RM produces results 12% (1.12) worse on average than SM. Indeed RM is better than SM in only one case ('uk', $P = 128$) and up to 33% worse ('dime20', $P = 128$) with the overall average quality 12% worse than SM. This is not altogether surprising since the AR of elements in the coarsest graph can be very poor if the matching takes no account of it, and hence the optimisation has to work with badly shaped elements. This limitation is graphically demonstrated in Figure 3 which shows an example of the shapes of the final 16 clusters in the coarsest graph of an example 2d mesh. Whilst the shapes for SM (3b) are very good (although the borders are somewhat irregular), the shapes for RM (3a) are extremely poor and as a result the partition optimisation on the coarser graphs is limited in the improvements that can be made.

When it comes to comparing SM with SCM & TCM (results not shown here, see [27]) there is actually very little difference; SCM is about 1.9% worse on average and TCM only about 0.6% worse. This suggests that the multilevel strategy is relatively robust to the matching algorithm *provided* the AR is taken into account in some way.

With regard to partitioning time, RM was on average about 32.9% slower than SM; as explained above this is because the optimisation is inhibited by the poor quality of the coarser graph and thus took considerably longer. SCM & TCM were about 14.3% & 8.5% slower than SM respectively; this is due to the slightly slower matching process. However the multilevel partitioning is generally very fast and any of the intelligent matching algorithms (as opposed to random matching, RM) do not add significantly to the optimisation time.

Overall this suggests that SM is the algorithm of choice although there is little benefit over TCM.

4 The Kernighan-Lin optimisation algorithm

In this section we outline the key features of an optimisation algorithm, fully described in [25] and then in §4.3 describe how it can be modified to optimise for AR. It is a Kernighan-Lin (KL) type algorithm incorporating a hill-climbing mechanism to enable it to escape from local minima. The algorithm uses bucket sorting, the linear time complexity improvement of Fiduccia & Mattheyses, [12], and is a partition optimisation formulation; in other words it optimises a partition of P subdomains rather than a bisection.

4.1 The gain function

A key concept in the method is the idea of *gain*. The gain $g(v,q)$ of a vertex v in subdomain S_p can be calculated for every other subdomain, S_q, $q \neq p$, and expresses how much the cost of a given partition would be improved were v to migrate to S_q. Thus, if π denotes the current partition and π' the partition if v migrates to S_q then for a cost function Γ, the gain $g(v,q) = \Gamma(\pi) - \Gamma(\pi')$. Assuming the migration of v only affects the cost of S_p and S_q (as is true for Γ_t and Γ_s) then from (1) we get

$$g(v,q) = \text{AR}(S_q) - \text{AR}(S_q + v) + \text{AR}(S_p) - \text{AR}(S_p - v). \quad (5)$$

For Γ_t this gives an expression

$$g_{\text{template}}(v,q) = \frac{1}{C}\left[\frac{\partial S_q}{(\Omega S_q)^{\frac{d-1}{d}}} - \frac{\partial\{S_q+v\}}{(\Omega\{S_q+v\})^{\frac{d-1}{d}}} + \frac{\partial S_p}{(\Omega S_p)^{\frac{d-1}{d}}} - \frac{\partial\{S_p-v\}}{(\Omega\{S_p-v\})^{\frac{d-1}{d}}}\right]. \quad (6)$$

which cannot be further simplified. However, for Γ_s, since

$$\begin{aligned}\text{AR}(S_q) - \text{AR}(S_q+v) &= \frac{1}{K_1}\left\{\partial^i S_q - \partial^i(S_q+v)\right\}\\ &= \frac{1}{K_1}\left\{\partial^i S_q \right.\\ &\quad \left. -(\partial^i S_q + \partial^i v - 2|(S_q,v)|)\right\}\\ &= \frac{1}{K_1}\left\{2|(S_q,v)| - \partial^i v\right\}\end{aligned}$$

(where $|(S_q,v)|$ denotes the sum of edge weights between S_q and v), we get

$$g_{\text{surface}}(v,q) = \frac{2}{K_1}\left\{|(S_q,v)| - |(S_p,v)|\right\} \quad (7)$$

Notice in particular that g_{surface} is the same as the cut-edge weight gain function and that it is entirely localised, i.e. the gain of a vertex only depends on the length of its boundaries with a subdomain and not on any intrinsic qualities of the subdomain which could be changed by non-local migration.

4.2 The iterative optimisation algorithm

The iterative optimisation algorithm, as is typical for KL type algorithms, has inner and outer iterative loops with the outer loop terminating when no migration takes place during an inner loop. The optimisation uses two bucket sorting structures or bucket trees, [25], and is initialised by calculating the gain for all border vertices and inserting them into one of the bucket trees. These vertices will subsequently be referred to as *candidate* vertices and the tree containing them as the *candidate tree*.

The inner loop proceeds by examining candidate vertices, highest gain first (by always picking vertices from the highest ranked bucket), testing whether the vertex is acceptable for migration and then transferring it to the other bucket tree (the tree of *examined* vertices). This inner loop terminates when the candidate tree is empty although it may terminate early if the partition cost rises too far above the cost of the best partition found so far. Once the inner loop has terminated any vertices remaining in the candidate tree are transferred to the examined tree and finally pointers to the two trees are swapped ready for the next pass through the inner loop.

The algorithm also uses a KL type hill-climbing strategy; in other words vertex migration from subdomain to subdomain can be *accepted* even if it degrades the partition quality and later, based on the subsequent evolution of the partition, either rejected or *confirmed*. During each pass through the inner loop, a record of the optimal partition achieved by migration within that loop is maintained together with a list of vertices which have migrated since that value was attained. If subsequent migration finds a 'better' partition then the migration is *confirmed* and the list is reset. Once the inner loop is terminated, any vertices remaining in the list (vertices whose migration has not been confirmed) are migrated back to the subdomains they came from when the optimal cost was attained.

The algorithm, together with conditions for vertex migration acceptance and confirmation is fully described in [25]. The impact of non-integer gain values on the bucket sorting is addressed and discussed in [27].

4.3 Incorporating aspect ratio: localisation

One of the advantages of using cut-edge weight as a cost function is its localised nature. When a graph vertex migrates from one subdomain to another, only the gains of adjacent vertices are affected. In contrast, when using the graph to optimise AR, if a vertex v migrates from S_p to S_q, the volume and surface of both subdomains will change. This in turn means that, when using the template cost function (2), the gain of all border vertices both within and abutting subdomains S_p and S_q will change. Strictly speaking, all these gains should be adjusted with the huge disadvantage that this may involve thousands of floating point operations and hence be prohibitively expensive. We have tested (Table 5) a version which includes full updating but, as alternatives, we propose three localised variants:

Surface Gain/Surface Cost (SGSC). The simplest way to localise the updating of the gains is to make the assumption in §2.2 that the subdomains all have approximately equal volume and to use the surface cost function Γ_s from (4). As mentioned in §2.3 the problem immediately reduces to the cut-edge weight problem, albeit with non-integer edge weights, and from (7) only the gains of the vertices adjacent to the migrating vertex will need updating. However, if this assumption is not true, it is not clear how well Γ_s will optimise the AR and below we discuss some experimental results.

Surface Gain/Template Cost (SGTC). The second method we propose for localising the updates of gain relies on the observation that the gain is simply used as a method of rating the vertices so that the algorithm always visits those with highest gain first (using the bucket sort). It is not clear how crucial this rating is to the success of the algorithm and indeed Karypis & Kumar demonstrated that (at least when optimising for cut-edge weight) almost as good results can be achieved by simply visiting the vertices in random order, [17]. We therefore propose approximating the gain with the surface cost function Γ_s from (4) to rate the vertices and store them in the bucket tree structure, but using the template cost function Γ_t from (2) to assess the change in cost when actually migrating an vertex. This localises the gain function.

Local Template Gain/Template Cost (LTGTC). A third possibility we propose is to actually use the template cost function, Γ_t for adjusting the gain, but only adjusting the gain of those vertices adjacent to the migrating vertex. The motivation is that the neighbours of the migrating vertex are likely to have large changes in gain whereas the gains of other vertices are

	$P=16$		$P=32$		$P=64$		$P=128$	
mesh	Γ_t	$\frac{\Gamma(\text{SGTC})-1}{\Gamma(\text{LTGTC})-1}$	Γ_t	$\frac{\Gamma(\text{SGTC})-1}{\Gamma(\text{LTGTC})-1}$	Γ_t	$\frac{\Gamma(\text{SGTC})-1}{\Gamma(\text{LTGTC})-1}$	Γ_t	$\frac{\Gamma(\text{SGTC})-1}{\Gamma(\text{LTGTC})-1}$
uk	1.62	1.00	1.50	1.08	1.41	1.03	1.40	1.00
4elt-dual	1.43	1.79	1.42	1.50	1.37	1.36	1.38	1.31
t60k	1.30	0.90	1.25	0.90	1.29	0.95	1.27	0.87
dime20	1.35	0.82	1.33	0.98	1.30	0.98	1.30	1.17
cs4	1.53	1.15	1.49	1.05	1.51	1.08	1.50	1.04
wing	1.65	1.74	1.65	1.65	1.66	1.62	1.63	1.46
mesh100	1.48	0.91	1.48	0.97	1.52	1.05	1.50	1.01
cyl3	1.52	1.10	1.52	0.99	1.53	1.03	1.52	1.02
Average		1.18		1.14		1.14		1.11

Table 4: Surface gain/template cost optimisation compared with local template gain/template cost

	$P=16$		$P=32$		$P=64$		$P=128$	
mesh	Γ_t	$\frac{\Gamma(\text{TGTC})-1}{\Gamma(\text{LTGTC})-1}$	Γ_t	$\frac{\Gamma(\text{TGTC})-1}{\Gamma(\text{LTGTC})-1}$	Γ_t	$\frac{\Gamma(\text{TGTC})-1}{\Gamma(\text{LTGTC})-1}$	Γ_t	$\frac{\Gamma(\text{TGTC})-1}{\Gamma(\text{LTGTC})-1}$
uk	1.64	1.04	1.49	1.06	1.38	0.95	1.38	0.96
4elt-dual	1.23	0.98	1.27	0.96	1.28	1.01	1.28	0.96
t60k	1.33	1.00	1.28	0.98	1.31	1.03	1.31	1.01
dime20	1.39	0.91	1.34	1.01	1.29	0.95	1.29	1.13
cs4	1.48	1.04	1.49	1.04	1.48	1.01	1.49	1.01
wing	1.38	1.01	1.41	1.04	1.41	1.00	1.44	1.02
mesh100	1.52	0.97	1.50	1.01	1.50	1.01	1.51	1.02
cyl3	1.48	1.02	1.51	0.98	1.52	1.01	1.52	1.02
Average		0.99		1.01		1.00		1.02

Table 5: Template gain/template cost optimisation compared with local template gain/template cost

likely to only change marginally (since they are only affected by the change in volume and surface of subdomains). The disadvantage is that the gains will become progressively more and more inaccurate as the optimisation progresses; however, they are still likely to be as accurate as using the surface cost.

Finally note that the implementation which, when a vertex migrates from subdomain S_p to S_q, involves full updating of the gains of all vertices in and adjacent to the borders of S_p and S_q is referred to as **Template Gain/Template Cost (TGTC)**.

4.4 Results for different optimisation functions

Table 4 compares SGTC optimisation against the LTGTC results from Table 2. Both sets of results use surface matching (SM). The table is in the same form as those in §3.3 and show that on average the surface gain function provides results which are 14.1% worse than LTGTC. Although we do not show the results here, a similar comparison shows that SGSC provides results which are 12.2% worse, [27].

Note that in earlier results, [26], we concluded that SGTC was the algorithm of choice and the reason for this discrepancy is explained in the test meshes used. In [26] we did not use the '4elt-dual' and 'wing' meshes which contain the highest mesh grading (the ratio of the largest surface of an element to the smallest), respectively 2.13e+4 and 1.08e+6. Looking at the results in more detail then '4elt-dual' gives average aspect ratios between 31-79% worse than LTGTC, while 'wing' ranges between 46-74% worse. These heavily influence the average results and the reason we believe this to happen is that the approximation (3) made in §2.2, that every subdomain has approximately equal volume, completely breaks down for meshes with very high gradings. For all the other meshes, the SGTC optimisation gives average ARs between 20% better to 17% worse than LTGTC and in fact, if we exclude the '4elt-dual' & 'wing' meshes from the results, on average SGTC is only 0.36% worse than LTGTC. This leads us to suggest that as a very rough 'ball park' figure, if the mesh grading is of the order 10^3 or less, the surface gain function provides perfectly good results, but if greater than this a more accurate estimate of gain is necessary and LTGTC is to be preferred.

Table 5 compares TGTC optimisation, the version which uses full updating of gains, with LTGTC and shows that on average LTGTC & TGTC give results which are almost equivalent in quality (TGTC is in fact 0.50% worse than LTGTC) and hence that LTGTC provides a very good approximation to TGTC.

Again we are not not primarily concerned with partitioning times, but it was interesting to note that SGSC & SGTC were on average 28.41% & 24.38% faster than LTGTC. This is because the surface cost function, Γ_s, is much quicker to calculate when assessing or updating the gains (since it does not involve calculating $S_p^{\frac{d-1}{d}}$). TGTC was over 50 times slower on average than LTGTC and we feel that this justifies the assertion that full updating of gains is too expensive.

Meanwhile in Table 7 we compare the edge cut produced by the EC version of JOSTLE with that of the AR version. As might be expected, EC partitioning produces the best results (about 14.4% better than AR). Notice, in particular, the results

	$P=16$		$P=32$		$P=64$		$P=128$	
mesh	Γ_t	$\frac{\Gamma(\text{EC})-1}{\Gamma(\text{AR})-1}$	Γ_t	$\frac{\Gamma(\text{EC})-1}{\Gamma(\text{AR})-1}$	Γ_t	$\frac{\Gamma(\text{EC})-1}{\Gamma(\text{AR})-1}$	Γ_t	$\frac{\Gamma(\text{EC})-1}{\Gamma(\text{AR})-1}$
uk	1.68	1.10	1.55	1.19	1.46	1.15	1.41	1.04
4elt-dual	1.32	1.33	1.28	1.01	1.29	1.06	1.29	1.01
t60k	1.38	1.13	1.31	1.09	1.33	1.09	1.32	1.02
dime20	1.50	1.17	1.45	1.33	1.40	1.33	1.38	1.45
cs4	1.52	1.12	1.54	1.15	1.53	1.12	1.51	1.05
wing	1.60	1.61	1.61	1.53	1.61	1.50	1.53	1.23
mesh100	1.55	1.03	1.60	1.22	1.61	1.24	1.61	1.21
cyl3	1.59	1.25	1.63	1.21	1.61	1.18	1.59	1.17
Average		1.22		1.22		1.21		1.15

Table 6: AR results for the edge cut partitioner compared with the AR partitioner

	$P=16$		$P=32$		$P=64$		$P=128$	
mesh	$\lvert E_c\rvert$	$\frac{\lvert E_c\rvert(\text{EC})}{\lvert E_c\rvert(\text{AR})}$	$\lvert E_c\rvert$	$\frac{\lvert E_c\rvert(\text{EC})}{\lvert E_c\rvert(\text{AR})}$	$\lvert E_c\rvert$	$\frac{\lvert E_c\rvert(\text{EC})}{\lvert E_c\rvert(\text{AR})}$	$\lvert E_c\rvert$	$\frac{\lvert E_c\rvert(\text{EC})}{\lvert E_c\rvert(\text{AR})}$
uk	182	0.92	305	0.92	512	0.92	809	0.86
4elt-dual	602	0.67	902	0.66	1515	0.76	2364	0.86
t60k	1016	0.99	1552	0.97	2439	0.97	3624	0.95
dime20	1382	0.73	2368	0.82	3717	0.80	5540	0.82
cs4	2496	0.95	3501	0.96	4666	0.93	6077	0.92
wing	5008	0.54	6866	0.50	9401	0.60	11877	0.70
mesh100	4782	0.79	7851	0.93	11100	0.96	15202	0.95
cyl3	11377	1.04	16783	1.02	22369	1.00	29432	0.98
Average		0.83		0.85		0.87		0.88

Table 7: $|E_c|$ results for the edge cut partitioner compared with the AR partitioner

for the 'wing' mesh (the mesh with the highest grading) where the EC partitioner produces partitions with up to 50% fewer cut edges than the AR partitioner, but the AR partitioner produces subdomains with aspect ratios 23-61% better. This demonstrates that a good partition for aspect ratio is not necessarily a good partition for edge-cut and vice-versa.

5 Discussion and conclusions

5.1 Comparison with cut-edge weight partitioning

In Table 6 we compare AR as produced by the edge cut version of JOSTLE (EC) described in [25] with the results from Table 2. The EC partitioner never produces average aspect ratios that are actually better than the AR partitioner and on average gives results which are 19.8% worse than those of the AR partitioner and can be up to 61% worse. Notice that there is no real consistency in the differences however (as there is in the differences between SGSC & SGTC compared with LTGTC – see §4.4) and we conclude that although an EC partitioner might be expected to produce reasonably good AR results (since a partition with a low value of $|E_c|$ is likely to have compact and therefore well shaped subdomains), targeting the cost function on AR can provide considerably better results in most cases.

In terms of time, the EC partitioner is about 2 times faster than AR on average. Again this is no surprise since the AR partitioning involves floating point operations (assessing cost and combining elements) while EC partitioning only requires integer operations. However both are extremely fast at producing high quality partitions.

5.2 Impact on solver iterations

To investigate the impact of different partitions on the convergence of a domain decomposition based preconditioner, we tested a solver on a number of partitions for two of the meshes. A heat distribution problem with Dirichlet boundary conditions was solved using the conjugate gradient algorithm supplied in the PETSC library [1] and the domain decomposition preconditioner implemented in the ParPre package [9]. Unfortunately, the parallel mesh environment we used, PadFEM, [6], is only implemented for 2d applications and so we were unable to test any 3d examples. In addition, limitations on the parallel hardware meant that we were only able to use up to 32 processors and the 'dime20' mesh was too large to fit into the memory; we also experienced some convergence problems with the '4elt-dual' mesh. However, the results presented in Table 8, where the partitions which have been optimised for aspect ratio always have fewer solver iterations, do confirm that the partition can have a significant impact on the convergence (and this is true even for a simple problem such as the Heat Equation – the effect may be magnified for more complex problems). More importantly for this paper, the results also suggest that the definition of aspect ratio used here can be a good cost function to optimise in order to enhance the convergence (although correlation between iterations and aspect ratio is somewhat tenuous).

		$P=8$			$P=16$			$P=32$		
mesh	optimisation	Γ_t	$\|E_c\|$	iterations	Γ_t	$\|E_c\|$	iterations	Γ_t	$\|E_c\|$	iterations
uk	AR	1.86	109	406	1.62	197	814	1.46	332	1029
uk	EC	1.91	99	571	1.68	182	873	1.55	305	1303
t60k	AR	1.32	569	2509	1.34	1031	2376	1.28	1607	4451
t60k	EC	1.33	539	2635	1.38	1016	2907	1.31	1552	5481

Table 8: The impact of partitions on the number of solver iterations

5.3 Generic multilevel mesh partitioning

In this paper we have adapted a mesh partitioning technique originally designed to solve the edge cut partitioning problem to a different cost function. The question then arises, is the multilevel strategy an appropriate technique for solving partitioning problems (or indeed other optimisation problems) with different cost functions? Clearly this is an impossible question to answer in general but a couple of pertinent remarks can be made:

- For the AR based cost functions at least, the method seems relatively sensitive to whether the cost is included in the matching. This suggests that, if possible, a generic multilevel partitioner should use the cost function to minimise the cost of the matchings. Note, however, that this may not be possible, since a cost function which, say, measured the cost of a mapping onto a particular processor topology would be unable to function since at the matching stage no partition, and hence no mapping exists.

- The optimisation relies, for efficiency at least, on having a local gain function in order that the migration of a vertex does not involve an $O(N/P)$ or even an $O(N)$ update. Here we were able to localise the updating of gains either by (a) making a simple approximation to localise the cost function, or (b) by just ignoring the updating of non-adjacent vertices. However, it is not clear that (a) is always possible or that (b) is always valid. On the other hand, the underlying approach in (a) which essentially decouples the gain from the cost does look quite promising for more general cost functions. In other words, we can use a local (and possibly crude) approximation for the gain function and then control the convergence/hill-climbing of the Kernighan Lin (KL) method, [18], with the true cost. In some ways, this could be regarded as a hybrid of the KL method and simulated annealing (SA), [19], because in some ways you could regard SA as KL with a random gain function. This concept of decoupling the gain and cost functions is part of our ongoing research.

5.4 Conclusion and future research

We have shown that the multilevel strategy can be modified to optimise for aspect ratio. In Section 2 we gave a definition of aspect ratio and showed how the graph could be modified to take AR into account. In Section 3.2 we described three matching algorithms (modifications of those already in the literature) which can be used to take AR into account and in Section 3.3 concluded that if it is not taken into account (i.e. random matching) the same quality of results cannot be expected. In Section 4.3 we described four ways of incorporating AR into a Kernighan-Lin based optimisation algorithm. We then demonstrated in Section 4.4 that we can approximate the cost function to localise the updating of gains reasonably successfully, provided that the mesh grading is not too high. We also showed that we can also localise the updating of gains by just ignoring non-adjacent vertices and concluded that full updating of gains does not provide any significant advantages (and costs a lot more). Finally in Sections 5.1 & 5.2 we showed that partitions with good subdomain aspect ratios can vary greatly from those with a low edge-cut and demonstrated on a subset of the meshes that our optimisation algorithm can indeed provide the convergence benefits for DD preconditioners that other researchers, using different definitions of aspect ratio, suggest, e.g. [10, 20, 23].

Finally, although a parallel version of JOSTLE exists, e.g. [28], it is not clear how well AR optimisation, with its more global cost function, will work in parallel and this is another direction for future research. Some related work on AR optimisation already exists in the context of a parallel dynamic adaptive mesh environment, [7, 8, 22], but none of this work involves multilevel methods so the question still arises whether parallel multilevel techniques can help in the optimisation.

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