

# SCOTCH and LIBSCOTCH 6.0 User's Guide

(version 6.0.4)

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#### Abstract

This document describes the capabilities and operations of SCOTCH and LIBSCOTCH, a software package and a software library devoted to static mapping, edge- and vertex-based graph partitioning, and sparse matrix block ordering of graphs and meshes/hypergraphs. It gives brief descriptions of the algorithms, details the input/output formats, instructions for use, installation procedures, and provides a number of examples.

SCOTCH is distributed as free/libre software, and has been designed such that new partitioning or ordering methods can be added in a straightforward manner. It can therefore be used as a testbed for the easy and quick coding and testing of such new methods, and may also be redistributed, as a library, along with third-party software that makes use of it, either in its original or in updated forms.

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# 1 Introduction

# 1.1 Static mapping

The efficient execution of a parallel program on a parallel machine requires that the communicating processes of the program be assigned to the processors of the machine so as to minimize its overall running time. When processes have a limited duration and their logical dependencies are accounted for, this optimization problem is referred to as *scheduling*. When processes are assumed to coexist simultaneously for the entire duration of the program, it is referred to as *mapping*. It amounts to balancing the computational weight of the processes among the processors of the machine, while reducing the cost of communication by keeping intensively inter-communicating processes on nearby processors. In most cases, the underlying computational structure of the parallel programs to map can be conveniently modeled as a graph in which vertices correspond to processes that handle distributed pieces of data, and edges reflect data dependencies. The mapping problem can then be addressed by assigning processor labels to the vertices of the graph, so that all

processes assigned to some processor are loaded and run on it. In a SPMD context, this is equivalent to the *distribution* across processors of the data structures of parallel programs; in this case, all pieces of data assigned to some processor are handled by a single process located on this processor.

A mapping is called *static* if it is computed prior to the execution of the program. Static mapping is NP-complete in the general case [14]. Therefore, many studies have been carried out in order to find sub-optimal solutions in reasonable time, including the development of specific algorithms for common topologies such as the hypercube [11, 22]. When the target machine is assumed to have a communication network in the shape of a complete graph, the static mapping problem turns into the *partitioning* problem, which has also been intensely studied [4, 23, 32, 34, 50]. However, when mapping onto parallel machines the communication network of which is not a bus, not accounting for the topology of the target machine usually leads to worse running times, because simple cut minimization can induce more expensive long-distance communication [22, 57].

# 1.2 Sparse matrix ordering

Many scientific and engineering problems can be modeled by sparse linear systems, which are solved either by iterative or direct methods. To achieve efficiency with direct methods, one must minimize the fill-in induced by factorization. This fill-in is a direct consequence of the order in which the unknowns of the linear system are numbered, and its effects are critical both in terms of memory and computation costs.

An efficient way to compute fill reducing orderings of symmetric sparse matrices is to use recursive nested dissection [18]. It amounts to computing a vertex set S that separates the graph into two parts A and B, ordering S with the highest indices that are still available, and proceeding recursively on parts A and B until their sizes become smaller than some threshold value. This ordering guarantees that, at each step, no non-zero term can appear in the factorization process between unknowns of A and unknowns of B.

The main issue of the nested dissection ordering algorithm is thus to find small vertex separators that balance the remaining subgraphs as evenly as possible, in order to minimize fill-in and to increase concurrency in the factorization process.

### 1.3 Contents of this document

This document describes the capabilities and operations of Scotch, a software package devoted to static mapping, graph and mesh partitioning, and sparse matrix block ordering. Scotch allows the user to map efficiently any kind of weighted process graph onto any kind of weighted architecture graph, and provides high-quality block orderings of sparse matrices. The rest of this manual is organized as follows. Section 2 presents the goals of the Scotch project. Sections 3 and 4 outline the most important aspects of the mapping and ordering algorithms that it implements, respectively. Section 5 summarizes the most important changes between version 5.0 and previous versions. Section 6 defines the formats of the files used in Scotch, section 7 describes the programs of the Scotch distribution, and section 8 defines the interface and operations of the LIBSCOTCH library. Section 9 explains how to obtain and install the Scotch distribution. Finally, some practical examples are given in section 10, and instructions on how to implement new methods in the LIBSCOTCH library are provided in section 11.

# 2 The Scotch project

# 2.1 Description

SCOTCH is a project carried out at the *Laboratoire Bordelais de Recherche en Informatique* (LaBRI) of the Université de Bordeaux and within the Bacchus teamproject of INRIA Bordeaux Sud-Ouest. Its goal is to study the application of graph theory to scientific computing.

It focused first on static mapping, and has resulted in the development of the Dual Recursive Bipartitioning (or DRB) mapping algorithm and in the study of several graph bipartitioning heuristics [42], all of which have been implemented in the SCOTCH software package [46]. Then, it focused on the computation of high-quality vertex separators for the ordering of sparse matrices by nested dissection, by extending the work that has been done on graph partitioning in the context of static mapping [47, 48]. The ordering capabilities of SCOTCH have then been extended to native mesh structures, thanks to hypergraph partitioning algorithms. Diffusion-based graph partitioning methods have also been added [8, 43].

Version 5.0 of Scotch was the first one to comprise parallel graph ordering routines. The parallel features of Scotch are referred to as PT-Scotch ("Parallel Threaded Scotch"). While both packages share a significant amount of code, because PT-Scotch transfers control to the sequential routines of the LIBSCOTCH library when the subgraphs on which it operates are located on a single processor, the two sets of routines have a distinct user's manual. Readers interested in the parallel features of Scotch should refer to the PT-Scotch 6.0 User's Guide [44].

Version 6.0 of Scotch is oriented towards the development of new features, namely graph repartitioning and remapping [13]. A whole set of direct k-way graph partitioning and mapping algorithms has also been implemented.

### 2.2 Availability

Starting from version 4.0, which has been developed at INRIA within the ScAlApplix project, Scotch is available under a dual licensing basis. On the one hand, it is downloadable from the Scotch web page as free/libre software, to all interested parties willing to use it as a library or to contribute to it as a testbed for new partitioning and ordering methods. On the other hand, it can also be distributed, under other types of licenses and conditions, to parties willing to embed it tightly into closed, proprietary software.

The free/libre software license under which SCOTCH 6.0 is distributed is the CeCILL-C license [6], which has basically the same features as the GNU LGPL ("Lesser General Public License"): ability to link the code as a library to any free/libre or even proprietary software, ability to modify the code and to redistribute these modifications. Version 4.0 of SCOTCH was distributed under the LGPL itself.

Please refer to section 9 to see how to obtain the free/libre distribution of Scotch.

# 3 Static mapping algorithms

The parallel program to be mapped onto the target architecture is modeled by a valuated unoriented graph S called source graph or process graph, the vertices of which represent the processes of the parallel program, and the edges of which the communication channels between communicating processes. Vertex- and edge- valuations associate with every vertex  $v_S$  and every edge  $e_S$  of S integer numbers  $w_S(v_S)$  and  $w_S(e_S)$  which estimate the computation weight of the corresponding process and the amount of communication to be transmitted on the channel, respectively.

The target machine onto which is mapped the parallel program is also modeled by a valuated unoriented graph T called  $target\ graph$  or  $architecture\ graph$ . Vertices  $v_T$  and edges  $e_T$  of T are assigned integer weights  $w_T(v_T)$  and  $w_T(e_T)$ , which estimate the computational power of the corresponding processor and the cost of traversal of the inter-processor link, respectively.

A mapping from S to T consists of two applications  $\tau_{S,T}:V(S)\longrightarrow V(T)$  and  $\rho_{S,T}:E(S)\longrightarrow \mathcal{P}(E(T))$ , where  $\mathcal{P}(E(T))$  denotes the set of all simple loopless paths which can be built from E(T).  $\tau_{S,T}(v_S)=v_T$  if process  $v_S$  of S is mapped onto processor  $v_T$  of T, and  $\rho_{S,T}(e_S)=\{e_T^1,e_T^2,\ldots,e_T^n\}$  if communication channel  $e_S$  of S is routed through communication links  $e_T^1,e_T^2,\ldots,e_T^n$  of T.  $|\rho_{S,T}(e_S)|$  denotes the dilation of edge  $e_S$ , that is, the number of edges of E(T) used to route  $e_S$ .

# 3.1 Cost function and performance criteria

The computation of efficient static mappings requires an  $a\ priori$  knowledge of the dynamic behavior of the target machine with respect to the programs which are run on it. This knowledge is synthesized in a  $cost\ function$ , the nature of which determines the characteristics of the desired optimal mappings. The goal of our mapping algorithm is to minimize some communication cost function, while keeping the load balance within a specified tolerance. The communication cost function  $f_C$  that we have chosen is the sum, for all edges, of their dilation multiplied by their weight:

$$f_C(\tau_{S,T}, \rho_{S,T}) \stackrel{\text{def}}{=} \sum_{e_S \in E(S)} w_S(e_S) \left| \rho_{S,T}(e_S) \right| .$$

This function, which has already been considered by several authors for hypercube target topologies [11, 22, 26], has several interesting properties: it is easy to compute, allows incremental updates performed by iterative algorithms, and its minimization favors the mapping of intensively intercommunicating processes onto nearby processors; regardless of the type of routing implemented on the target machine (store-and-forward or cut-through), it models the traffic on the interconnection network and thus the risk of congestion.

The strong positive correlation between values of this function and effective execution times has been experimentally verified by Hammond [22] on the CM-2, and by Hendrickson and Leland [27] on the nCUBE 2.

The quality of mappings is evaluated with respect to the criteria for quality that we have chosen: the balance of the computation load across processors, and the minimization of the inter-processor communication cost modeled by function  $f_C$ . These criteria lead to the definition of several parameters, which are described below.

For load balance, one can define  $\mu_{map}$ , the average load per computational power unit (which does not depend on the mapping), and  $\delta_{map}$ , the load imbalance ratio, as

$$\mu_{map} \stackrel{\text{def}}{=} \frac{\sum\limits_{v_S \in V(S)} w_S(v_S)}{\sum\limits_{v_T \in V(T)} w_T(v_T)} \quad \text{and}$$

$$\sum\limits_{v_T \in V(T)} \left| \left( \frac{1}{w_T(v_T)} \sum\limits_{\substack{v_S \in V(S) \\ \tau_{S,T}(v_S) = v_T}} w_S(v_S) \right) - \mu_{map} \right| \\ \sum\limits_{v_S \in V(S)} w_S(v_S) \quad .$$

However, since the maximum load imbalance ratio is provided by the user in input of the mapping, the information given by these parameters is of little interest, since what matters is the minimization of the communication cost function under this load balance constraint.

For communication, the straightforward parameter to consider is  $f_C$ . It can be normalized as  $\mu_{exp}$ , the average edge expansion, which can be compared to  $\mu_{dil}$ , the average edge dilation; these are defined as

the average edge dilation; these are defined as 
$$\mu_{exp} \stackrel{\text{def}}{=} \frac{f_C}{\sum\limits_{e_S \in E(S)} w_S(e_S)} \quad \text{and} \quad \mu_{dil} \stackrel{\text{def}}{=} \frac{\sum\limits_{e_S \in E(S)} |\rho_{S,T}(e_S)|}{|E(S)|} \ .$$

 $\delta_{exp} \stackrel{\text{def}}{=} \frac{\mu_{exp}}{\mu_{dil}}$  is smaller than 1 when the mapper succeeds in putting heavily intercommunicating processes closer to each other than it does for lightly communicating processes; they are equal if all edges have same weight.

# 3.2 The Dual Recursive Bipartitioning algorithm

This mapping algorithm, which is the primary way to compute initial static mappings, uses a divide and conquer approach to recursively allocate subsets of processes to subsets of processors [42, 45]. It starts by considering a set of processors, also called domain, containing all the processors of the target machine, and with which is associated the set of all the processes to map. At each step, the algorithm bipartitions a yet unprocessed domain into two disjoint subdomains, and calls a graph bipartitioning algorithm to split the subset of processes associated with the domain across the two subdomains, as sketched in the following.

The association of a subdomain with every process defines a *partial mapping* of the process graph. As bipartitionings are performed, the subdomain sizes decrease, up to give a complete mapping when all subdomains are of size one.

The above algorithm lies on the ability to define five main objects:

- a domain structure, which represents a set of processors in the target architecture;
- a domain bipartitioning function, which, given a domain, bipartitions it in two disjoint subdomains;
- a domain distance function, which gives, in the target graph, a measure of the distance between two disjoint domains. Since domains may not be convex nor connected, this distance may be estimated. However, it must respect certain homogeneity properties, such as giving more accurate results as domain sizes decrease. The domain distance function is used by the graph bipartitioning algorithms to compute the communication function to minimize, since it allows the mapper to estimate the dilation of the edges that link vertices which belong to different domains. Using such a distance function amounts to considering that all routings will use shortest paths on the target architecture, which is how most parallel machines actually do. We have thus chosen that our program would not provide routings for the communication channels, leaving their handling to the communication system of the target machine;
- a process subgraph structure, which represents the subgraph induced by a subset of the vertex set of the original source graph;
- a process subgraph bipartitioning function, which bipartitions subgraphs in two disjoint pieces to be mapped onto the two subdomains computed by the domain bipartitioning function.

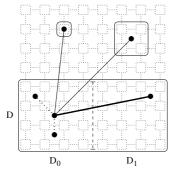
All these routines are seen as black boxes by the mapping program, which can thus accept any kind of target architecture and process bipartitioning functions.

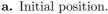
### 3.2.1 Partial cost function

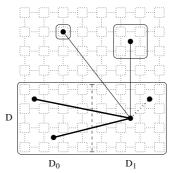
The production of efficient complete mappings requires that all graph bipartitionings favor the criteria that we have chosen. Therefore, the bipartitioning of a subgraph S' of S should maintain load balance within the user-specified tolerance, and minimize the *partial* communication cost function  $f'_C$ , defined as

$$f'_{C}(\tau_{S,T}, \rho_{S,T}) \stackrel{\text{def}}{=} \sum_{\substack{v \in V(S') \\ \{v, v'\} \in E(S)}} w_{S}(\{v, v'\}) |\rho_{S,T}(\{v, v'\})| ,$$

which accounts for the dilation of edges internal to subgraph S' as well as for the one of edges which belong to the cocycle of S', as shown in Figure 1. Taking into account the partial mapping results issued by previous bipartitionings makes it possible to avoid local choices that might prove globally bad, as explained below. This amounts to incorporating additional constraints to the standard graph bipartitioning problem, turning it into a more general optimization problem termed skewed graph partitioning by some authors [28].







**b.** After one vertex is moved.

Figure 1: Edges accounted for in the partial communication cost function when bipartitioning the subgraph associated with domain D between the two subdomains  $D_0$  and  $D_1$  of D. Dotted edges are of dilation zero, their two ends being mapped onto the same subdomain. Thin edges are cocycle edges.

#### 3.2.2 Execution scheme

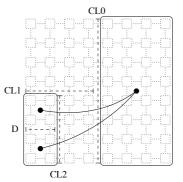
From an algorithmic point of view, our mapper behaves as a greedy algorithm, since the mapping of a process to a subdomain is never reconsidered, and at each step of which iterative algorithms can be applied. The double recursive call performed at each step induces a recursion scheme in the shape of a binary tree, each vertex of which corresponds to a bipartitioning job, that is, the bipartitioning of both a domain and its associated subgraph.

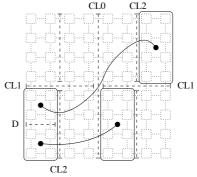
In the case of depth-first sequencing, as written in the above sketch, bipartitioning jobs run in the left branches of the tree have no information on the distance between the vertices they handle and neighbor vertices to be processed in the right branches. On the contrary, sequencing the jobs according to a by-level (breadth-first) travel of the tree allows any bipartitioning job of a given level to have information on the subdomains to which all the processes have been assigned at the previous level. Thus, when deciding in which subdomain to put a given process, a bipartitioning job can account for the communication costs induced by its neighbor processes, whether they are handled by the job itself or not, since it can estimate in  $f'_C$  the dilation of the corresponding edges. This results in an interesting feedback effect: once an edge has been kept in a cut between two subdomains, the distance between its end vertices will be accounted for in the partial communication cost function to be minimized, and following jobs will be more likely to keep these vertices close to each other, as illustrated in Figure 2. The relative efficiency of depth-first and breadth-first sequencing schemes with respect to the structure of the source and target graphs is discussed in [45].

# 3.2.3 Clustering by mapping onto variable-sized architectures

Several constrained graph partitioning problems can be modeled as mapping the problem graph onto a target architecture, the number of vertices and topology of which depend dynamically on the structure of the subgraphs to bipartition at each step.

Variable-sized architectures are supported by the DRB algorithm in the following way: at the end of each bipartitioning step, if any of the variable subdomains is empty (that is, all vertices of the subgraph are mapped only to one of the subdomains), then the DRB process stops for both subdomains, and all of the vertices





- a. Depth-first sequencing.
- **b.** Breadth-first sequencing.

Figure 2: Influence of depth-first and breadth-first sequencings on the bipartitioning of a domain D belonging to the leftmost branch of the bipartitioning tree. With breadth-first sequencing, the partial mapping data regarding vertices belonging to the right branches of the bipartitioning tree are more accurate (C.L. stands for "Cut Level").

are assigned to their parent subdomain; else, if a variable subdomain has only one vertex mapped onto it, the DRB process stops for this subdomain, and the vertex is assigned to it.

The moment when to stop the DRB process for a specific subgraph can be controlled by defining a bipartitioning strategy that checks the validity of a criterion at each bipartitioning step (see for instance Section 8.15.2), and maps all of the subgraph vertices to one of the subdomains when it becomes false.

## 3.3 Static mapping methods

The core of our static mapping software uses graph mapping methods as black boxes. It maintains an internal image of the current mapping, which records the target vertex index onto which each of the source graph vertices is mapped. It is therefore possible to apply several mapping methods in sequence, such that the first method computes an initial mapping to be further refined by the following methods, thus enabling us to define *static mapping strategies*. The currently implemented static mapping methods are listed below.

# Multilevel

This framework, which has been studied by several authors [4, 24, 32] and should be considered as a strategy rather than as a method since it uses other methods as parameters, repeatedly reduces the size of the graph to map by finding matchings that collapse vertices and edges, computes a mapping of the coarsest graph obtained, and prolongs the result back to the original graph, as shown in Figure 3. The multilevel method, when used in conjunction with some local optimization methods to refine the projected partitions at every level, usually leads to a significant improvement in quality with respect to methods operating only on the finest graph. By coarsening the graphs, the multilevel algorithm broadens the scope of local optimization algorithms: it makes possible for them to account for topological structures of the original graph that would else be of a too high level for them to be encompassed in their local optimization process.

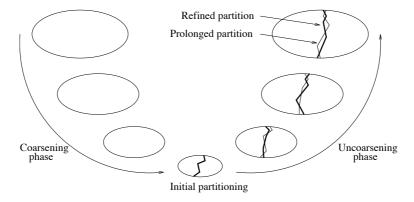


Figure 3: The multilevel partitioning process. In the uncoarsening phase, the light and bold lines represent for each level the prolonged partition obtained from the coarser graph, and the partition obtained after refinement, respectively.

### Band

Like the multilevel method above, the band method is a framework, in the sense that it does not itself compute partitions, but rather helps other partitioning algorithms perform better. It is a refinement algorithm which, from a given initial partition, extracts a band graph of given width (which only contains graph vertices that are at most at this distance from the frontiers of the parts), calls a partitioning strategy on this band graph, and projects back the refined partition on the original graph. This method was designed to be able to use expensive partitioning heuristics, such as genetic algorithms, on large graphs, as it dramatically reduces the problem space by several orders of magnitude. However, it was found that, in a multilevel context, it also improves partition quality, by coercing partitions in a problem space that derives from the one which was globally defined at the coarsest level, thus preventing local optimization refinement algorithms to be trapped in local optima of the finer graphs [8].

## Fiduccia-Mattheyses

This is a direct k-way version of the traditional Fiduccia-Mattheyses heuristics used for computing bipartitions, that will be presented in the next section. By default, boundary vertices can only be moved to parts to which at least one of their neighbors belong.

### Diffusion

This is also a k-way version of an algorithm that has been first used in the context of bipartitioning, and which will be presented in the next section. The k-way version differs from the latter as it diffuses k sorts of liquids rather than just two as in the bipartitioning case.

### Exactifier

This greedy algorithm refines its input mapping so as to reduce load imbalance as much as possible. Since this method does not consider load balance minimization, its use should be restricted to cases where achieving load balance is critical and where recursive bipartitioning may fail to achieve it. It is especially the case when vertex loads are very irregular: some subdomains may receive only a few heavy vertices, yielding load balance artifacts when no light vertices are locally available to compensate.

Graph vertices are sorted by decreasing weights, and considered in turn. If the current vertex can fit in its initial part without causing imbalance by excess, it is added to it, and the algorithm goes on. Else, a candidate part is found by exploring other subdomains in an order based on an implicit recursive bipartitioning of the architecture graph. Consequently, such vertices will be placed in subdomains that tend to be as close as possible to the original location of the vertex. This method is most likely to result in disconnected parts.

### Dual recursive bipartitioning

This algorithm implements the dual recursive bipartitioning algorithm that has been presented in Section 3.2. The DRB algorithms can be used either directly on the original graph to partition, or on the coarsest graph yielded by the direct k-way multilevel framework. It uses graph bipartitioning methods, described below, to compute its bipartitions.

# 3.4 Graph bipartitioning methods

The core of our dual recursive bipartitioning mapping algorithm uses process graph bipartitioning methods as black boxes. It allows the mapper to run any type of graph bipartitioning method compatible with our criteria for quality. Bipartitioning jobs maintain an internal image of the current bipartition, indicating for every vertex of the job whether it is currently assigned to the first or to the second subdomain. It is therefore possible to apply several different methods in sequence, each one starting from the result of the previous one, and to select the methods with respect to the job characteristics, thus enabling us to define graph bipartitioning strategies. The currently implemented graph bipartitioning methods are listed below.

### Diffusion

This global optimization method, presented in [43], flows two kinds of antagonistic liquids, scotch and anti-scotch, from two source vertices, and sets the new frontier as the limit between vertices which contain scotch and the ones which contain anti-scotch. In order to add load-balancing constraints to the algorithm, a constant amount of liquid disappears from every vertex per unit of time, so that no domain can spread across more than half of the vertices. Because selecting the source vertices is essential to the obtainment of useful results, this method has been hard-coded so that the two source vertices are the two vertices of highest indices, since in the band method these are the anchor vertices which represent all of the removed vertices of each part. Therefore, this method must be used on band graphs only, or on specifically crafted graphs.

### Exactifier

This greedy algorithm refines the current partition so as to reduce load imbalance as much as possible, while keeping the value of the communication cost function as small as possible. The vertex set is scanned in order of decreasing vertex weights, and vertices are moved from one subdomain to the other if doing so reduces load imbalance. When several vertices have same weight, the vertex whose swap decreases most the communication cost function is selected first. This method is used in post-processing of other methods when load balance is mandatory. For weighted graphs, the strict enforcement of load balance may cause the swapping of isolated vertices of small weight, thus

greatly increasing the cut. Therefore, great care should be taken when using this method if connectivity or cut minimization are mandatory.

### Fiduccia-Mattheyses

The Fiduccia-Mattheyses heuristics [12] is an almost-linear improvement of the famous Kernighan-Lin algorithm [36]. It tries to improve the bipartition that is input to it by incrementally moving vertices between the subsets of the partition, as long as it can find sequences of moves that lower its communication cost. By considering sequences of moves instead of single swaps, the algorithm allows hill-climbing from local minima of the cost function. As an extension to the original Fiduccia-Mattheyses algorithm, we have developed new data structures, based on logarithmic indexings of arrays, that allow us to handle weighted graphs while preserving the almost-linearity in time of the algorithm [45].

As several authors quoted before [25, 33], the Fiduccia-Mattheyses algorithm gives better results when trying to optimize a good starting partition. Therefore, it should not be used on its own, but rather after greedy starting methods such as the Gibbs-Poole-Stockmeyer or the greedy graph growing methods.

### Gibbs-Poole-Stockmeyer

This greedy bipartitioning method derives from an algorithm proposed by Gibbs, Poole, and Stockmeyer to minimize the dilation of graph orderings, that is, the maximum absolute value of the difference between the numbers of neighbor vertices [19]. The graph is sliced by using a breadth-first spanning tree rooted at a randomly chosen vertex, and this process is iterated by selecting a new root vertex within the last layer as long as the number of layers increases. Then, starting from the current root vertex, vertices are assigned layer after layer to the first subdomain, until half of the total weight has been processed. Remaining vertices are then allocated to the second subdomain.

As for the original Gibbs, Poole, and Stockmeyer algorithm, it is assumed that the maximization of the number of layers results in the minimization of the sizes—and therefore of the cocycles— of the layers. This property has already been used by George and Liu to reorder sparse linear systems using the nested dissection method [18], and by Simon in [55].

### Greedy graph growing

This greedy algorithm, which has been proposed by Karypis and Kumar [32], belongs to the GRASP ("Greedy Randomized Adaptive Search Procedure") class [37]. It consists in selecting an initial vertex at random, and repeatedly adding vertices to this growing subset, such that each added vertex results in the smallest increase in the communication cost function. This process, which stops when load balance is achieved, is repeated several times in order to explore (mostly in a gradient-like fashion) different areas of the solution space, and the best partition found is kept.

# Multilevel

This is a graph bipartition-oriented version of the static mapping multilevel method described in the previous section, page 13.

# 4 Sparse matrix ordering algorithms

When solving large sparse linear systems of the form Ax = b, it is common to precede the numerical factorization by a symmetric reordering. This reordering is chosen in such a way that pivoting down the diagonal in order on the resulting permuted matrix  $PAP^T$  produces much less fill-in and work than computing the factors of A by pivoting down the diagonal in the original order (the fill-in is the set of zero entries in A that become non-zero in the factored matrix).

# 4.1 Performance criteria

The quality of orderings is evaluated with respect to several criteria. The first one, NNZ, is the number of non-zero terms in the factored reordered matrix. The second one, OPC, is the operation count, that is the number of arithmetic operations required to factor the matrix. The operation count that we have considered takes into consideration all operations (additions, subtractions, multiplications, divisions) required by Cholesky factorization, except square roots; it is equal to  $\sum_c n_c^2$ , where  $n_c$  is the number of non-zeros of column c of the factored matrix, diagonal included. A third criterion for quality is the shape of the elimination tree; concurrency in parallel solving is all the higher as the elimination tree is broad and short. To measure its quality, several parameters can be defined:  $h_{\min}$ ,  $h_{\max}$ , and  $h_{\text{avg}}$  denote the minimum, maximum, and average heights of the tree<sup>1</sup>, respectively, and  $h_{\text{dlt}}$  is the variance, expressed as a percentage of  $h_{\text{avg}}$ . Since small separators result in small chains in the elimination tree,  $h_{\text{avg}}$  should also indirectly reflect the quality of separators.

# 4.2 Minimum Degree

The minimum degree algorithm [56] is a local heuristic that performs its pivot selection by iteratively selecting from the graph a node of minimum degree.

The minimum degree algorithm is known to be a very fast and general purpose algorithm, and has received much attention over the last three decades (see for example [1, 17, 40]). However, the algorithm is intrinsically sequential, and very little can be theoretically proved about its efficiency.

### 4.3 Nested dissection

The nested dissection algorithm [18] is a global, heuristic, recursive algorithm which computes a vertex set S that separates the graph into two parts A and B, ordering S with the highest remaining indices. It then proceeds recursively on parts A and B until their sizes become smaller than some threshold value. This ordering guarantees that, at each step, no non zero term can appear in the factorization process between unknowns of A and unknowns of B.

Many theoretical results have been carried out on nested dissection ordering [7, 39], and its divide and conquer nature makes it easily parallelizable. The main issue of the nested dissection ordering algorithm is thus to find small vertex separators that balance the remaining subgraphs as evenly as possible. Most often, vertex separators are computed by using direct heuristics [29, 38], or from edge separators [49, and included references] by minimum cover techniques [9, 31], but other techniques such as spectral vertex partitioning have also been used [50].

 $<sup>^{1}</sup>$ We do not consider as leaves the disconnected vertices that are present in some meshes, since they do not participate in the solving process.

Provided that good vertex separators are found, the nested dissection algorithm produces orderings which, both in terms of fill-in and operation count, compare favorably [20, 32, 47] to the ones obtained with the minimum degree algorithm [40]. Moreover, the elimination trees induced by nested dissection are broader, shorter, and better balanced, and therefore exhibit much more concurrency in the context of parallel Cholesky factorization [3, 15, 16, 20, 47, 54, and included references].

# 4.4 Hybridization

Due to their complementary nature, several schemes have been proposed to hybridize the two methods [29, 35, 47]. However, to our knowledge, only loose couplings have been achieved: incomplete nested dissection is performed on the graph to order, and the resulting subgraphs are passed to some minimum degree algorithm. This results in the fact that the minimum degree algorithm does not have exact degree values for all of the boundary vertices of the subgraphs, leading to a misbehavior of the vertex selection process.

Our ordering program implements a tight coupling of the nested dissection and minimum degree algorithms, that allows each of them to take advantage of the information computed by the other. First, the nested dissection algorithm provides exact degree values for the boundary vertices of the subgraphs passed to the minimum degree algorithm (called *halo* minimum degree since it has a partial visibility of the neighborhood of the subgraph). Second, the minimum degree algorithm returns the assembly tree that it computes for each subgraph, thus allowing for supervariable amalgamation, in order to obtain column-blocks of a size suitable for BLAS3 block computations.

As for our mapping program, it is possible to combine ordering methods into ordering strategies, which allow the user to select the proper methods with respect to the characteristics of the subgraphs.

The ordering program is completely parametrized by its ordering strategy. The nested dissection method allows the user to take advantage of all of the graph partitioning routines that have been developed in the earlier stages of the SCOTCH project. Internal ordering strategies for the separators are relevant in the case of sequential or parallel [21, 51, 52, 53] block solving, to select ordering algorithms that minimize the number of extra-diagonal blocks [7], thus allowing for efficient use of BLAS3 primitives, and to reduce inter-processor communication.

# 4.5 Ordering methods

The core of our ordering algorithm uses graph ordering methods as black boxes, which allows the orderer to run any type of ordering method. In addition to yielding orderings of the subgraphs that are passed to them, these methods may compute column block partitions of the subgraphs, that are recorded in a separate tree structure. The currently implemented graph ordering methods are listed below.

### Halo approximate minimum degree

The halo approximate minimum degree method [48] is an improvement of the approximate minimum degree [1] algorithm, suited for use on subgraphs produced by nested dissection methods. Its interest compared to classical minimum degree algorithms is that boundary vertices are processed using their real degree in the global graph rather than their (much smaller) degree in the subgraph, resulting in smaller fill-in and operation count. This method also implements amalgamation techniques that result in efficient block computations in the factoring and the solving processes.

### Halo approximate minimum fill

The halo approximate minimum fill method is a variant of the halo approximate minimum degree algorithm, where the criterion to select the next vertex to permute is not based on its current estimated degree but on the minimization of the induced fill.

# Graph compression

The graph compression method [2] merges cliques of vertices into single nodes, so as to speed-up the ordering of the compressed graph. It also results in some improvement of the quality of separators, especially for stiffness matrices.

# Gibbs-Poole-Stockmeyer

This method is mainly used on separators to reduce the number and extent of extra-diagonal blocks.

### Simple method

Vertices are ordered consecutively, in the same order as they are stored in the graph. This is the fastest method to use on separators when the shape of extra-diagonal structures is not a concern.

### Nested dissection

Incomplete nested dissection method. Separators are computed recursively on subgraphs, and specific ordering methods are applied to the separators and to the resulting subgraphs (see sections 4.3 and 4.4).

## 4.6 Graph separation methods

The core of our incomplete nested dissection algorithm uses graph separation methods as black boxes. It allows the orderer to run any type of graph separation method compatible with our criteria for quality, that is, reducing the size of the vertex separator while maintaining the loads of the separated parts within some user-specified tolerance. Separation jobs maintain an internal image of the current vertex separator, indicating for every vertex of the job whether it is currently assigned to one of the two parts, or to the separator. It is therefore possible to apply several different methods in sequence, each one starting from the result of the previous one, and to select the methods with respect to the job characteristics, thus enabling the definition of separation strategies.

The currently implemented graph separation methods are listed below.

### Fiduccia-Mattheyses

This is a vertex-oriented version of the original, edge-oriented, Fiduccia-Mattheyses heuristics described in page 16.

### Greedy graph growing

This is a vertex-oriented version of the edge-oriented greedy graph growing algorithm described in page 16.

#### Multilevel

This is a vertex-oriented version of the edge-oriented multilevel algorithm described in page 13.

#### Thinner

This greedy algorithm refines the current separator by removing all of the exceeding vertices, that is, vertices that do not have neighbors in both parts. It is provided as a simple gradient refinement algorithm for the multilevel method, and is clearly outperformed by the Fiduccia-Mattheyses algorithm.

#### Vertex cover

This algorithm computes a vertex separator by first computing an edge separator, that is, a bipartition of the graph, and then turning it into a vertex separator by using the method proposed by Pothen and Fang [49]. This method requires the computation of maximal matchings in the bipartite graphs associated with the edge cuts, which are built using Duff's variant [9] of the Hopcroft and Karp algorithm [31]. Edge separators are computed by using a bipartitioning strategy, which can use any of the graph bipartitioning methods described in section 3.4, page 15.

# 5 Updates

# 5.1 Changes from version 5.0

A new integer index type has been created in the Fortran interface, to address array indices larger than the maximum value which can be stored in a regular integer. Please refer to Section 9.3 for more information.

A new set of routines has been designed, to ease the use of the LIBSCOTCH as a dynamic library. The SCOTCH\_version routine returns the version, release and patch level numbers of the library being used. The SCOTCH\_\*Alloc routines, which are only available in the C interface at the time being, dynamically allocate storage space for the opaque API SCOTCH structures, which frees application programs from the need to be systematically recompiled because of possible changes of SCOTCH structure sizes.

# 5.2 Changes from version 5.1

Direct k-way graph partitioning and static mapping methods are now available. They are less expensive than the classical dual recursive bipartitioning scheme, and improve quality on average for numbers of parts above a few hundreds. Another new method aims at reducing load imbalance in the case of source graphs with highly irregular vertex weights; see Section 3.3, page 13. Users willing to keep using the old recursive bipartitioning strategies of the 5.x branch can create default strategies with the SCOTCH\_STRATRECURSIVE flag set, in addition to other flags; see Section 8.3.1, page 59 for further information.

Graph repartitioning and static re-mapping features are now available; see Sections 8.7.2 to 8.7.7, starting from page 93.

The clustering capabilities of Scotch can be used more easily from the command line and library calls; see Section 7.3.6 and Section 8.15.2.

A new set of routines has been created in order to compute vertex-separated, k-way partitions, that balance the loads of the parts and of the separator vertices that surround them; see Sections 8.3.4 and 8.7.5.

A new labeled tree-leaf architecture has been created, for nodes that label cores in non increasing order. See Section 6.4.2, page 26 for the description of the ltleaf target architecture.

Memory footprint measurement routines are now available to users; see Section 8.19, page 145.

Key algorithms are now multi-threaded. See the installation file INSTALL.txt in the main directory for instructions on how to compile SCOTCH with thread support enabled.

# 6 Files and data structures

For the sake of portability, readability, and reduction of storage space, all the data files shared by the different programs of the SCOTCH project are coded in plain ASCII text exclusively. Although we may speak of "lines" when describing file formats, text-formatting characters such as newlines or tabulations are not mandatory, and are not taken into account when files are read. They are only used to provide better readability and understanding. Whenever numbers are used to label objects, and unless explicitly stated, **numberings always start from zero**, not one.

# 6.1 Graph files

Graph files, which usually end in ".grf" or ".src", describe valuated graphs, which can be valuated process graphs to be mapped onto target architectures, or graphs representing the adjacency structures of matrices to order.

Graphs are represented by means of adjacency lists: the definition of each vertex is accompanied by the list of all of its neighbors, i.e. all of its adjacent arcs. Therefore, the overall number of edge data is twice the number of edges.

Since version 3.3 has been introduced a new file format, referred to as the "new-style" file format, which replaces the previous, "old-style", file format. The two advantages of the new-style format over its predecessor are its greater compacity, which results in shorter I/O times, and its ability to handle easily graphs output by C or by Fortran programs.

Starting from version 4.0, only the new format is supported. To convert remaining old-style graph files into new-style graph files, one should get version 3.4 of the SCOTCH distribution, which comprises the scv file converter, and use it to produce new-style SCOTCH graph files from the old-style SCOTCH graph files which it is able to read. See section 7.3.5 for a description of gcv, formerly called scv.

The first line of a graph file holds the graph file version number, which is currently 0. The second line holds the number of vertices of the graph (referred to as vertnbr in LIBSCOTCH; see for instance Figure 16, page 54, for a detailed example), followed by its number of arcs (unappropriately called edgenbr, as it is in fact equal to twice the actual number of edges). The third line holds two figures: the graph base index value (baseval), and a numeric flag.

The graph base index value records the value of the starting index used to describe the graph; it is usually 0 when the graph has been output by C programs, and 1 for Fortran programs. Its purpose is to ease the manipulation of graphs within each of these two environments, while providing compatibility between them.

The numeric flag, similar to the one used by the Chaco graph format [25], is made of three decimal digits. A non-zero value in the units indicates that vertex weights are provided. A non-zero value in the tenths indicates that edge weights are provided. A non-zero value in the hundredths indicates that vertex labels are

provided; if it is the case, vertices can be stored in any order in the file; else, natural order is assumed, starting from the graph base index.

This header data is then followed by as many lines as there are vertices in the graph, that is, vertnbr lines. Each of these lines begins with the vertex label, if necessary, the vertex load, if necessary, and the vertex degree, followed by the description of the arcs. An arc is defined by the load of the edge, if necessary, and by the label of its other end vertex. The arcs of a given vertex can be provided in any order in its neighbor list. If vertex labels are provided, vertices can also be stored in any order in the file.

Figure 4 shows the contents of a graph file modeling a cube with unity vertex and edge weights and base 0.

0			
8	24		
0	000		
3	4	2	1
3	5	3	0
3	6	0	3
3	7	1	2
3	0	6	5
3	1	7	4
3	2	4	7
3	3	5	6

Figure 4: Graph file representing a cube.

# 6.2 Mesh files

Mesh files, which usually end in ".msh", describe valuated meshes, made of elements and nodes, the elements of which can be mapped onto target architectures, and the nodes of which can be reordered.

Meshes are bipartite graphs, in the sense that every element is connected to the nodes that it comprises, and every node is connected to the elements to which it belongs. No edge connects any two element vertices, nor any two node vertices. One can also think of meshes as hypergraphs, such that nodes are the vertices of the hypergraph and elements are hyper-edges which connect multiple nodes, or reciprocally such that elements are the vertices of the hypergraph and nodes are hyper-edges which connect multiple elements.

Since meshes are graphs, the structure of mesh files resembles very much the one of graph files described above in section 6.1, and differs only by its header, which indicates which of the vertices are node vertices and element vertices.

The first line of a mesh file holds the mesh file version number, which is currently 1. Graph and mesh version numbers will always differ, which enables application programs to accept both file formats and adapt their behavior according to the type of input data. The second line holds the number of elements of the mesh (velmnbr), followed by its number of nodes (vnodnbr), and by its overall number of arcs (edgenbr, that is, twice the number of edges which connect elements to nodes and vice-versa).

The third line holds three figures: the base index of the first element vertex in memory (velmbas), the base index of the first node vertex in memory (vnodbas), and a numeric flag.

The SCOTCH mesh file format requires that all nodes and all elements be assigned to contiguous ranges of indices. Therefore, either all element vertices are defined before all node vertices, or all node vertices are defined before all element vertices. The node and element base indices indicate at the same time whether elements or nodes are put in the first place, as well as the value of the starting index used to describe the graph. Indeed, if velmbas < vnodbas, then elements have the smallest indices, velmbas is the base value of the underlying graph (that is, baseval = velmbas), and velmbas + velmnbr = vnodbas holds. Conversely, if velmbas > vnodbas, then nodes have the smallest indices, vnodbas is the base value of the underlying graph, (that is, baseval = vnodbas), and vnodbas+vnodnbr = velmbas holds.

The numeric flag, similar to the one used by the CHACO graph format [25], is made of three decimal digits. A non-zero value in the units indicates that vertex weights are provided. A non-zero value in the tenths indicates that edge weights are provided. A non-zero value in the hundredths indicates that vertex labels are provided; if it is the case, and if velmbas < vnodbas (resp. velmbas > vnodbas), the velmbr (resp. vnodbr) first vertex lines are assumed to be element (resp. node) vertices, irrespective of their vertex labels, and the vnodnbr (resp. velmnbr) remaining vertex lines are assumed to be node (resp. element) vertices; else, natural order is assumed, starting at the underlying graph base index (baseval).

This header data is then followed by as many lines as there are node and element vertices in the graph. These lines are similar to the ones of the graph format, except that, in order to save disk space, the numberings of nodes and elements all start from the same base value, that is, min(velmbas, vnodbas) (also called baseval, like for regular graphs).

For example, Figure 5 shows the contents of the mesh file modeling three square elements, with unity vertex and edge weights, elements defined before nodes, and numbering of the underlying graph starting from 1. In memory, the three elements are labeled from 1 to 3, and the eight nodes are labeled from 4 to 11. In the file, the three elements are still labeled from 1 to 3, while the eight nodes are labeled from 1 to 8.

When labels are used, elements and nodes may have similar labels, but not two elements, nor two nodes, should have the same labels.

# 6.3 Geometry files

Geometry files, which usually end in ".xyz", hold the coordinates of the vertices of their associated graph or mesh. These files are not used in the mapping process itself, since only topological properties are taken into account then (mappings are computed regardless of graph geometry). They are used by visualization programs to compute graphical representations of mapping results.

The first string to appear in a geometry file codes for its type, or dimensionality. It is "1" if the file contains unidimensional coordinates, "2" for bidimensional coordinates, and "3" for tridimensional coordinates. It is followed by the number of coordinate data stored in the file, which should be at least equal to the number of vertices of the associated graph or mesh, and by that many coordinate lines. Each coordinate line holds the label of the vertex, plus one, two or three real numbers which are the (X), (X,Y), or (X,Y,Z), coordinates of the graph vertices, according to the graph dimensionality.

Vertices can be stored in any order in the file. Moreover, a geometry file can have more coordinate data than there are vertices in the associated graph or mesh file:

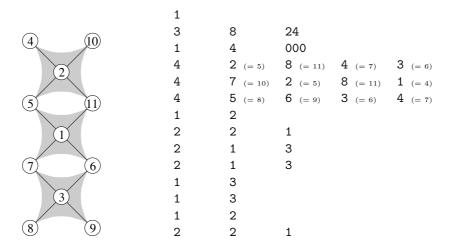


Figure 5: Mesh file representing three square elements, with unity vertex and edge weights. Elements are defined before nodes, and numbering of the underlying graph starts from 1. The left part of the figure shows the mesh representation in memory, with consecutive element and node indices. The right part of the figure shows the contents of the file, with both element and node numberings starting from 1, the minimum of the element and node base values. Corresponding node indices in memory are shown in parentheses for the sake of comprehension.

only coordinates the labels of which match labels of graph or mesh vertices will be taken into account. This feature allows all subgraphs of a given graph or mesh to share the same geometry file, provided that graph vertex labels remain unchanged. For example, Figure 6 shows the contents of the 3D geometry file associated with the graph of Figure 4.

3			
8			
0	0.0	0.0	0.0
1	0.0	0.0	1.0
2	0.0	1.0	0.0
3	0.0	1.0	1.0
4	1.0	0.0	0.0
5	1.0	0.0	1.0
6	1.0	1.0	0.0
7	1.0	1.0	1.0

Figure 6: Geometry file associated with the graph file of Figure 4.

# 6.4 Target files

Target files describe the architectures onto which source graphs are mapped. Instead of containing the structure of the target graph itself, as source graph files do, target files define how target graphs are bipartitioned and give the distances between all pairs of vertices (that is, processors). Keeping the bipartitioning information within target files avoids recomputing it every time a target architecture is used. We are allowed to do so because, in our approach, the recursive bipartitioning of the target graph is fully independent with respect to that of the source graph (however, the opposite is false).

For space and time saving issues, some classical homogeneous architectures (2D and 3D meshes and tori, hypercubes, complete graphs, etc.) have been algorithmically coded within the mapper itself by the means of built-in functions. Instead of containing the whole graph decomposition data, their target files hold only a few values, used as parameters by the built-in functions.

### 6.4.1 Decomposition-defined architecture files

Decomposition-defined architecture files are the standard way to describe weighted and/or irregular target architectures. Several file formats exist, but we only present here the most humanly readable one, which begins in "deco 0" ("deco" stands for "decomposition-defined" architecture, and "0" is the format type).

The "deco 0" header is followed by two integer numbers, which are the number of processors and the largest terminal number used in the decomposition, respectively. Two arrays follow. The first array has as many lines as there are processors. Each of these lines holds three numbers: the processor label, the processor weight (that is an estimation of its computational power), and its terminal number. The terminal number associated with every processor is obtained by giving the initial domain holding all the processors number 1, and by numbering the two subdomains of a given domain of number i with numbers 2i and 2i + 1. The second array is a lower triangular diagonal-less matrix that gives the distance between all pairs of processors. This distance matrix, combined with the decomposition tree coded by terminal numbers, allows the evaluation by averaging of the distance between all pairs of domains. In order for the mapper to behave properly, distances between processors must be strictly positive numbers. Therefore, null distances are not accepted. For instance, Figure 7 shows the contents of the architecture decomposition file for UB(2,3), the binary de Bruijn graph of dimension 3, as computed by the amk\_grf program.

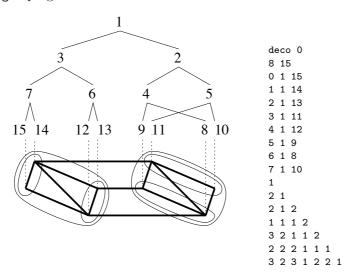


Figure 7: Target decomposition file for UB(2,3). The terminal numbers associated with every processor define a unique recursive bipartitioning of the target graph.

### 6.4.2 Algorithmically-coded architecture files

Almost all algorithmically-coded architectures are defined with unity edge and vertex weights. They start with an abbreviation name of the architecture, followed by parameters specific to the architecture. The available built-in architecture definitions are listed below.

#### ${\tt cmplt}\ size$

Defines a complete graph with size vertices. Its vertex labels are numbers between 0 and size - 1.

### cmpltw size $load_0$ $load_1$ ... $load_{size-1}$

Defines a weighted complete graph with size vertices. Its vertex labels are numbers between 0 and size - 1, and vertices are assigned integer weights in the order in which these are provided.

#### hcub dim

Defines a binary hypercube of dimension dim. Graph vertices are numbered according to the value of the binary representation of their coordinates in the hypercube.

# tleaf lev lnbr $size val_0$ $link val_0$ ... $size val_{lev lnbr-1}$ $link val_{lev lnbr-1}$

Defines a hierarchical, tree-shaped, architecture with levlnbr levels and  $\sum_{i=0}^{levlnbr-1} sizeval_i$  leaf vertices. This topology is used to model hierarchical NUMA or NUIOA machines. The mapping is only computed with respect to the leaf vertices, which represent processing elements, while the upper levels of the tree model interconnection networks (intra-chip buses, inter-chip interconnection networks, network routers, etc.), as exemplified in Figure 8. The communication cost between two nodes is the cost of the highest common ancestor level.

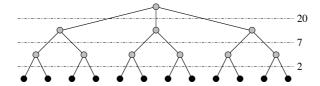


Figure 8: A "tree-leaf" graph with three levels. Processors are drawn in black and routers in grey. The description of this architecture is "tleaf 3 3 20 2 7 2 2". It has 3 levels, the first level has 3 sons and a traversal cost of 20, the second level has 2 sons and a traversal cost of 7, and the third level has also 2 sons and a traversal cost of 2.

ltleaf levlnbr  $sizeval_0$   $linkval_0$  ...  $sizeval_{levlnbr-1}$   $linkval_{levlnbr-1}$  permnbr  $permval_0$  ...  $permval_{permnbr-1}$ 

The ltleaf (for "labeled tree-leaf") architecture is an extended tree-leaf architecture which models target topologies where cores are not labeled in increasing order.

The tree structure of the architecture is described just like for a regular tleaf architecture. permnbr is the length of the permutation that is used to label cores, followed by this number of permutation indices, ranging between 0 and (permnbr-1). Figure 9 presents an example of such an architecture.

The permutation array must be of a size that matches level boundaries. Alternatively, a permutation of size 1, with only index 0 given, represents the identity permutation. In this case, the regular tleaf architecture can be used.

```
ltleaf
3 32 10 2 5 4 1
8 0 2 4 6 1 3 5 7
```

Figure 9: Labeled tree-leaf architecture with 3 levels, representing a system with 32 nodes of 2 quad-core processors. Inter-node communication costs 10, inter-processor communication within the same node costs 5 and inter-core communication within the same processor costs 1. Within a 8-core node, cores are labeled such that cores 0, 2, 4 and 6 are located on the first processor, while cores 1, 3, 5 and 7 are located on the second processor.

#### $mesh2D \ dim X \ dim Y$

Defines a bidimensional array of dimX columns by dimY rows. The vertex with coordinates (posX, posY) has label  $posY \times dimX + posX$ .

### mesh3D $dim X \ dim Y \ dim Z$

Defines a tridimensional array of dimX columns by dimY rows by dimZ levels. The vertex with coordinates (posX, posY, posZ) has label  $(posZ \times dimY + posY) \times dimX + posX$ .

### torus2D dim X dim Y

Defines a bidimensional array of dimX columns by dimY rows, with wraparound edges. The vertex with coordinates (posX, posY) has label  $posY \times dimX + posX$ .

### torus3D $dim X \ dim Y \ dim Z$

Defines a tridimensional array of dimX columns by dimY rows by dimZ levels, with wraparound edges. The vertex with coordinates (posX, posY, posZ) has label  $(posZ \times dimY + posY) \times dimX + posX$ .

### 6.4.3 Variable-sized architecture files

Variable-sized architectures are a class of algorithmically-coded architectures the size of which is not defined *a priori*. Domains of these target architectures can always be bipartitioned, again and again (until integer overflow occurs in domain indices). These architectures are used to perform graph clustering (see Sections 7.3.6 and 8.7.1), using a specifically tailored graph mapping strategy (see for instance Section 8.15.2).

As for fixed-size algorithmically-coded architectures, they start with an abbreviation name of the architecture, followed by parameters specific to the architecture. The available built-in variable-sized architecture definitions are listed below.

### varcmplt

Defines a variable-sized complete graph. Domains are labeled such that the first domain is labeled 1, and the two subdomains of any domain i are labeled 2i and 2i + 1. The distance between any two subdomains i and j is 0 if i = j and 1 else.

varhcub

Defines a variable-sized hypercube. Domains are labeled such that the first domain is labeled 1, and the two subdomains of any domain i are labeled 2i and 2i+1. The distance between any two domains is the Hamming distance between the common bits of the two domains, plus half of the absolute difference between the levels of the two domains, this latter term modeling the average distance on unknown bits. For instance, the distance between subdomain  $9=1001_B$ , of level 3 (since its leftmost 1 has been shifted left thrice), and subdomain  $53=110101_B$ , of level 5 (since its leftmost 1 has been shifted left five times), is equal to 2: it is 1, which is the number of bits which differ between  $1101_B$  (that is,  $53=110101_B$  shifted rightwards twice) and  $1001_B$ , plus 1, which is half of the absolute difference between 5 and 3.

# 6.5 Mapping files

Mapping files, which usually end in ".map", contain the result of the mapping of source graphs onto target architectures. They associate a vertex of the target graph with every vertex of the source graph.

Mapping files begin with the number of mapping lines which they contain, followed by that many mapping lines. Each mapping line holds a mapping pair, made of two integer numbers which are the label of a source graph vertex and the label of the target graph vertex onto which it is mapped. Mapping pairs can be stored in any order in the file; however, labels of source graph vertices must be all different. For example, Figure 10 shows the result obtained when mapping the source graph of Figure 4 onto the target architecture of Figure 7. This one-to-one embedding of H(3) into UB(2,3) has dilation 1, except for one hypercube edge which has dilation 3.

Figure 10: Mapping file obtained when mapping the hypercube source graph of Figure 4 onto the binary de Bruijn architecture of Figure 7.

Mapping files are also used on output of the block orderer to represent the allocation of the vertices of the original graph to the column blocks associated with the ordering. In this case, column blocks are labeled in ascending order, such that the number of a block is always greater than the ones of its predecessors in the elimination process, that is, its leaves in the elimination tree.

# 6.6 Ordering files

Ordering files, which usually end in ".ord", contain the result of the ordering of source graphs or meshes that represent sparse matrices. They associate a number with every vertex of the source graph or mesh.

The structure of ordering files is analogous to the one of mapping files; they differ only by the meaning of their data.

Ordering files begin with the number of ordering lines which they contain, that is the number of vertices in the source graph or the number of nodes in the source mesh, followed by that many ordering lines. Each ordering line holds an ordering pair, made of two integer numbers which are the label of a source graph or mesh vertex and its rank in the ordering. Ranks range from the base value of the graph or mesh (baseval) to the base value plus the number of vertices (resp. nodes), minus one (baseval + vertnbr -1 for graphs, and baseval + vnodnbr -1 for meshes). Ordering pairs can be stored in any order in the file; however, indices of source vertices must be all different.

For example, Figure 11 shows the result obtained when reordering the source graph of Figure 4.

Figure 11: Ordering file obtained when reordering the hypercube graph of Figure 4.

The advantage of having both graph and mesh orderings start from baseval (and not vnodbas in the case of meshes) is that an ordering computed on the nodal graph of some mesh has the same structure as an ordering computed from the native mesh structure, allowing for greater modularity. However, in memory, permutation indices for meshes are numbered from vnodbas to vnodbas + vnodnbr - 1.

# 6.7 Vertex list files

Vertex lists are used by programs that select vertices from graphs.

Vertex lists are coded as lists of integer numbers. The first integer is the number of vertices in the list and the other integers are the labels of the selected vertices, given in any order. For example, Figure 12 shows the list made from three vertices of labels 2, 45, and 7.

3 2 45 7

Figure 12: Example of vertex list with three vertices of labels 2, 45, and 7.

# 7 Programs

The programs of the Scotch project belong to five distinct classes.

- Graph handling programs, the names of which begin in "g", that serve to build and test source graphs.
- Mesh handling programs, the names of which begin in "m", that serve to build and test source meshes.

- Target architecture handling programs, the names of which begin in "a", that allow the user to build and test decomposition-defined target files, and especially to turn a source graph file into a target file.
- The mapping and ordering programs themselves.
- Output handling programs, which are the mapping performance analyzer, the graph factorization program, and the graph, matrix, and mapping visualization program.

The general architecture of the Scotch project is displayed in Figure 13.

### 7.1 Invocation

The programs comprising the SCOTCH project have been designed to run in command-line mode without any interactive prompting, so that they can be called easily from other programs by means of "system()" or "popen()" system calls, or be piped together on a single shell command line. In order to facilitate this, whenever a stream name is asked for (either on input or output), the user may put a single "-" to indicate standard input or output. Moreover, programs read their input in the same order as stream names are given in the command line. It allows them to read all their data from a single stream (usually the standard input), provided that these data are ordered properly.

A brief on-line help is provided with all the programs. To get this help, use the "-h" option after the program name. The case of option letters is not significant, except when both the lower and upper cases of a letter have different meanings. When passing parameters to the programs, only the order of file names is significant; options can be put anywhere in the command line, in any order. Examples of use of the different programs of the Scotch project are provided in section 10.

Error messages are standardized, but may not be fully explanatory. However, most of the errors you may run into should be related to file formats, and located in "...Load" routines. In this case, compare your data formats with the definitions given in section 6, and use the gtst and mtst programs to check the consistency of source graphs and meshes.

# 7.2 Using compressed files

Starting from version 5.0.6, SCOTCH allows users to provide and retrieve data in compressed form. Since this feature requires that the compression and decompression tasks run in the same time as data is read or written, it can only be done on systems which support multi-threading (Posix threads) or multi-processing (by means of fork system calls).

To determine if a stream has to be handled in compressed form, SCOTCH checks its extension. If it is ".gz" (gzip format), ".bz2" (bzip2 format) or ".lzma" (lzma format), the stream is assumed to be compressed according to the corresponding format. A filter task will then be used to process it accordingly if the format is implemented in SCOTCH and enabled on your system.

To date, data can be read and written in bzip2 and gzip formats, and can also be read in the lzma format. Since the compression ratio of lzma on SCOTCH graphs is 30% better than the one of gzip and bzip2 (which are almost equivalent in this case), the lzma format is a very good choice for handling very large graphs. To see how to enable compressed data handling in SCOTCH, please refer to Section 9.

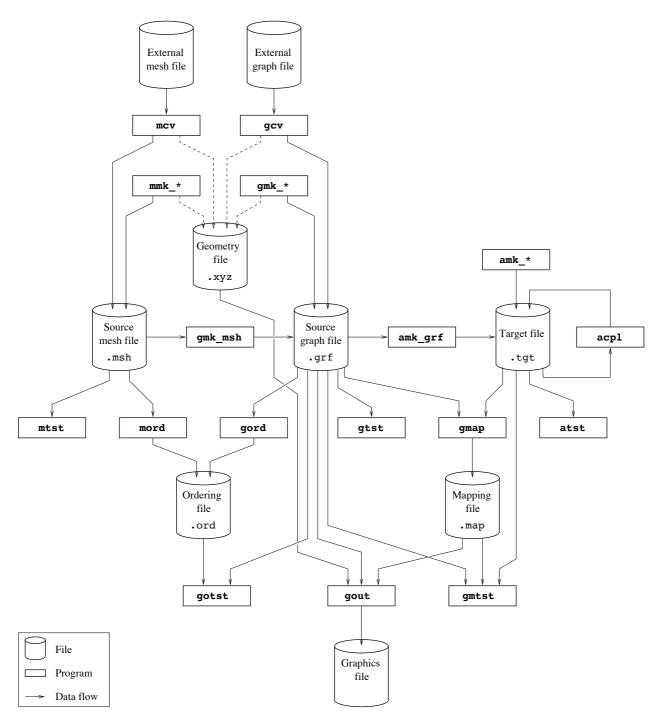


Figure 13: General architecture of the Scotch project. All of the features offered by the stand-alone programs are also available in the LIBSCOTCH library.

When the compressed format allows it, several files can be provided on the same stream, and be uncompressed on the fly. For instance, the command "cat brol.grf.gz brol.xyz.gz | gout -.gz -.gz -Mn - brol.iv" concatenates the topology and geometry data of some graph brol and feed them as a single compressed stream to the standard input of program gout, hence the "-.gz" to indicate a compressed standard stream.

# 7.3 Description

# 7.3.1 acpl

# Synopsis

acpl [input\_target\_file [output\_target\_file]] options

### Description

The program acpl is the decomposition-defined architecture file compiler. It processes architecture files of type "deco 0" built by hand or by the amk\_\* programs, to create a "deco 1" compiled architecture file of about four times the size of the original one; see section 6.4.1, page 25, for a detailed description of decomposition-defined target architecture file formats.

The mapper can read both original and compiled architecture file formats. However, compiled architecture files are read much more efficiently, as they are directly loaded into memory without further processing. Since the compilation time of a target architecture graph evolves as the square of its number of vertices, precompiling with acpl can save some time when many mappings are to be performed onto the same large target architecture.

# Options

- -h Display the program synopsis.
- -V Print the program version and copyright.

# 7.3.2 amk\_\*

### Synopsis

```
amk_ccc dim [output_target_file] options

amk_fft2 dim [output_target_file] options

amk_hy dim [output_target_file] options

amk_m2 dimX [dimY [output_target_file]] options

amk_p2 weight0 [weight1 [output_target_file]] options
```

### Description

The amk\_\* programs make target graphs. Each of them is devoted to a specific topology, for which it builds target graphs of any dimension.

These programs are an alternate way between algorithmically-coded built-in

target architectures and decompositions computed by mapping with amk\_grf. Like built-in target architectures, their decompositions are algorithmically computed, and like amk\_grf, their output is a decomposition-defined target architecture file. These programs allow the definition and testing of new algorithmically-coded target architectures without coding them in the core of the mapper.

Program amk\_ccc outputs the target architecture file of a Cube-Connected-Cycles graph of dimension dim. Vertex (l,m) of CCC(dim), with  $0 \le l < dim$  and  $0 \le m < 2^{dim}$ , is linked to vertices  $((l-1) \mod dim, m)$ ,  $((l+1) \mod dim, m)$ , and  $(l, m \oplus 2^l)$ , and is labeled  $l \times 2^{dim} + m$ .  $\oplus$  denotes the bitwise exclusive-or binary operator, and  $a \mod b$  the integer remainder of the euclidian division of a by b.

Program amk\_fft2 outputs the target architecture file of a binary Fast-Fourier-Transform graph of dimension dim. Vertex (l,m) of FFT(dim), with  $0 \le l \le dim$  and  $0 \le m < 2^{dim}$ , is linked to vertices (l-1,m),  $(l-1,m \bmod 2^{l-1})$ , (l+1,m), and  $(l+1,m \oplus 2^l)$ , if they exist, and is labeled  $l \times 2^{dim} + m$ .

Program amk\_hy outputs the target architecture file of a hypercube graph of dimension dim. Vertices are labeled according to the decimal value of their binary representation. The decomposition-defined target architectures computed by amk\_hy do not exactly give the same results as the built-in hypercube targets because distances are not computed in the same manner, although the two recursive bipartitionings are identical. To achieve best performance and save space, use the built-in architecture.

Program amk\_p2 outputs the target architecture file of a weighted path graph with two vertices, the weights of which are given as parameters.

This simple target topology is used to bipartition a source graph into two weighted parts with as few cut edges as possible. In particular, it is used to compute independent partitions of the processors of a multi-user parallel machine. As a matter of fact, if the yet unallocated part of the machine is represented by a source graph with n vertices, and n' processors are requested by a user in order to run a job (with  $n' \leq n$ ), mapping the source graph onto the weighted path graph with two vertices of weights n' and n-n' leads to a partition of the machine in which the allocated n' processors should be as densely connected as possible (see Figure 14).

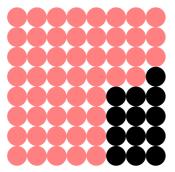
## Options

-h Display the program synopsis.

-mmethod

Select the bipartitioning method (for amk\_m2 only).

- n Nested dissection.
- Dimension-per-dimension one-way dissection. This is less efficient than nested dissection, and this feature exists only for benchmarking purposes.
- -V Print the program version and copyright.



a. Construction of a partition with 13 vertices (in black) on a  $8 \times 8$  bidimensional mesh architecture.



**b.** Construction of a partition with 17 vertices (in black) on the remaining architecture.

Figure 14: Construction of partitions on a bidimensional  $8 \times 8$  mesh architecture by weighted bipartitioning.

#### 7.3.3 amk\_grf

## **Synopsis**

 $amk\_grf[input\_graph\_file[output\_target\_file]] options$ 

### Description

The program amk\_grf turns a source graph file into a decomposition-defined target file. It computes a recursive bipartitioning of the source graph, as well as the array of distances between all pairs of its vertices, both of which are combined to give a decomposition-defined target architecture of same topology as the input source graph.

The -1 option restricts the target architecture to the vertices indicated in the given vertex list file. It is therefore possible to build a target architecture made of several disconnected parts of a bigger architecture. Note that this is not equivalent to turning a disconnected source graph into a target architecture, since doing so would lead to an architecture made of several independent pieces at infinite distance one from another. Considering the selected vertices within their original architecture makes it possible to compute the distance between vertices belonging to distinct connected components, and therefore to evaluate the cost of the mapping of two neighbor processes onto disjoint areas of the architecture.

The restriction feature is very useful in the context of multi-user parallel machines. On these machines, when users request processors in order to run their jobs, the partitions allocated by the operating system may not be regular nor connected, because of existing partitions already attributed to other people. By feeding <code>amk\_grf</code> with the source graph representing the whole parallel machine, and the vertex list containing the labels of the processors allocated by the operating system, it is possible to build a target architecture corresponding to this partition, and therefore to map processes on it, automatically, regardless of the partition shape.

The -b option selects the recursive bipartitioning strategy used to build the decomposition of the source graph. For regular, unweighted, topologies, the '-b(g|h)fx' recursive bipartitioning strategy should work best. For irregular

or weighted graphs, use the default strategy, which is more flexible. See also the manual page of function SCOTCH\_archBuild, page 78, for further information.

# Options

#### -bstrategy

Use recursive bipartitioning strategy strategy to build the decomposition of the architecture graph. The format of bipartitioning strategies is defined within section 8.3.2, at page 63.

- -h Display the program synopsis.
- -linput\_vertex\_file

Load vertex list from *input\_vertex\_file*. As for all other file names, "-" may be used to indicate standard input.

-V Print the program version and copyright.

#### 7.3.4 atst

## Synopsis

atst [input\_target\_file [output\_data\_file]] options

## Description

The program atst is the architecture tester. It gives some statistics on decomposition-defined target architectures, and in particular the minimum, maximum, and average communication costs (that is, weighted distance) between all pairs of processors.

### **Options**

- -h Display the program synopsis.
- -V Print the program version and copyright.

### 7.3.5 gcv

### Synopsis

gcv [input\_graph\_file [output\_graph\_file [output\_geometry\_file]]] options

### Description

The program gcv is the source graph converter. It takes on input a graph file of the format specified with the -i option, and outputs its equivalent in the format specified with the -o option, along with its associated geometry file whenever geometry data is available. At the time being, it accepts four input formats: the Matrix Market format [5], the Harwell-Boeing collection format [10], the Chaco/MeTiS graph format [25], and the Scotch format. Three output format are available: the Matrix Market format, the Chaco/MeTiS graph format and the Scotch source graph and geometry data format.

# Options

-h Display the program synopsis.

### -iformat

Specify the type of input graph. The available input formats are listed below.

# b[number]

Harwell-Boeing graph collection format. Only symmetric assembled matrices are currently supported. Since files in this format can contain several graphs one after another, the optional integer number, starting from 0, indicates which graph of the file is considered for conversion.

- c Chaco v1.0/MeTiS format.
- m The Matrix Market format.
- s Scotch source graph format.

#### -oformat

Specify the output graph format. The available output formats are listed below.

- c Chaco v1.0/MeTiS format.
- m The Matrix Market format.
- s Scotch source graph format.
- -V Print the program version and copyright.

Default option set is "-Ib0 -0s".

# **7.3.6** gmap / gpart

## Synopsis

 $\begin{tabular}{ll} $\tt gmap [input\_graph\_file [input\_target\_file [output\_mapping\_file [output\_log\_file]]]] options \end{tabular}$ 

 $\begin{tabular}{ll} {\bf gpart} & number\_of\_parts & [input\_graph\_file & [output\_mapping\_file & [output\_log\_file]]] \\ options & \\ \end{tabular}$ 

#### Description

The program gmap is the graph mapper. It uses a partitioning strategy to map a source graph onto a target graph, so that the weight of source graph vertices allocated to target vertices is balanced, and the communication cost function  $f_C$  is minimized.

The program **gpart** is the graph partitioner. It uses a partitioning strategy to split a source graph into the prescribed number of parts, using vertex or edge separators, depending whether the -o option is set or not.

The implemented mapping methods mainly derive from graph theory. In particular, graph geometry is never used, even if it is available; only topological properties are taken into account. Mapping methods are used to define mapping strategies by means of selection, combination, grouping, and condition operators.

Mapping methods implemented in version 6.0 comprise direct k-way methods, including a k-way multilevel framework and k-way local refinement methods, as well as the Dual Recursive Bipartitioning algorithm, which uses graph

bipartitioning methods. Available bipartitioning methods include a multilevel framework that uses other bipartitioning methods to compute the initial and refined bipartitions: an improved implementation of the Fiduccia–Mattheyses heuristic designed to handle weighted graphs, a diffusion-based algorithm, a greedy method derived from the Gibbs, Poole, and Stockmeyer algorithm, a greedy graph growing heuristic, a greedy "exactifying" refinement algorithm designed to balance vertex loads as much as possible, etc.

gpart is a simplified interface to gmap, which performs graph partitioning instead of static mapping. Consequently, the desired number of parts has to be provided, in lieu of the target architecture.

The -b and -c options allow the user to set preferences on the behavior of the mapping strategy which is used by default. The -m option allows the user to define a custom mapping strategy.

Both programs can be used to perform clustering, by means of the -q option. gpart will perform topology-independent clustering, while gmap may compute locality-preserving clusters when mapping onto variable-sized, non-complete, architectures (see Section 6.4.3).

If mapping statistics are wanted rather than the mapping output itself, mapping output can be set to /dev/null, with option -vmt to get mapping statistics and timings.

### **Options**

Since the program is devoted to experimental studies, it has many optional parameters, used to test various execution modes. Values set by default will give best results in most cases.

#### -b rat

Set the maximum load imbalance ratio to rat, which should be a value comprised between 0 and 1. This option can be used in conjunction with option -c, but is incompatible with option -m.

## -cflags

Tune the default mapping strategy according to the given preference flags. Some of these flags are antagonistic, while others can be combined. See Section 8.3.1 for more information. The currently available flags are the following.

- b Enforce load balance as much as possible.
- q Privilege quality over speed.
- ${\tt r}$  Only use recursive bipartitioning methods.
- s Privilege speed over quality.
- t Use only safe methods in the strategy.

This option can be used in conjunction with option -b, but is incompatible with option -m. The resulting strategy string can be displayed by means of the -vs option.

-h Display the program synopsis.

### -mstrat

Apply mapping strategy *strat*. In the case of static mapping or of edgebased graph partitioning, the format of mapping strategies should comply with the format defined in Section 8.3.2. If the -o option is used (see below), strategies must be vertex partitioning strategies, which are described in Section 8.3.4. This option is incompatible with options -b and -c.

-o Compute vertex-based partitions rather than static mappings or edgebased partitions. This option is only valid for gpart, or when gmap is called with a target architecture which is an unweighted complete graph.

### -q (for gpart)

# -qpwght

(for gmap) Perform clustering instead of partitioning or mapping. Clustering is achieved by means of a specific strategy string that performs recursive bipartitioning until the size of the parts is smaller than some threshold value. For gpart, this value replaces the desired number of parts as the first argument passed to the program. For gmap, the threshold must be given just after the -q option.

#### -sobj

Mask source edge and vertex weights. This option allows the user to "unweight" weighted source graphs by removing weights from edges and vertices at loading time. *obj* may contain several of the following switches.

- e Remove edge weights, if any.
- v Remove vertex weights, if any.
- -V Print the program version and copyright.

#### -vverb

Set verbose mode to *verb*, which may contain several of the following switches. For a detailed description of the data displayed, please refer to the manual page of gmtst below.

- Mapping or partitioning information, depending whether the -o option has been set or not.
- s Strategy information. This parameter displays the mapping strategy which will be used by gmap or gpart.
- t Timing information.
- -V Print the program version and copyright.

### 7.3.7 gmk\_\*

#### **Synopsis**

```
gmk_hy dim [output\_graph\_file] options gmk_m2 dimX [dimY [output\_graph\_file]] options gmk_m3 dimX [dimY [dimZ [output\_graph\_file]]] options gmk_ub2 dim [output\_graph\_file] options
```

### Description

The gmk\_\* programs make source graphs. Each of them is devoted to a specific topology, for which it builds target graphs of any dimension.

The gmk\_\* programs are mainly used in conjunction with amk\_grf. Most gmk\_\* programs build source graphs describing parallel machines, which

are used by <code>amk\_grf</code> to generate corresponding target sub-architectures, by means of its <code>-l</code> option. Such a procedure is shown in section 10, which builds a target architecture from five vertices of a binary de Bruijn graph of dimension 3.

Program gmk\_hy outputs the source file of a hypercube graph of dimension dim. Vertices are labeled according to the decimal value of their binary representation.

Program  $gmk_m2$  outputs the source file of a bidimensional mesh with dimX columns and dimY rows. If the -t option is set, tori are built instead of meshes. The vertex of coordinates (posX, posY) is labeled  $posY \times dimX + posX$ .

Program gmk\_m3 outputs the source file of a tridimensional mesh with dimZ layers of dimY rows by dimX columns. If the -t option is set, tori are built instead of meshes. The vertex of coordinates (posX, posY) is labeled  $(posZ \times dimY + posY) \times dimX + posX$ .

Program gmk\_ub2 outputs the source file of a binary unoriented de Bruijn graph of dimension dim. Vertices are labeled according to the decimal value of their binary representation.

## Options

-goutput\_geometry\_file

Output graph geometry to file <code>output\_geometry\_file</code> (for <code>gmk\_m2</code> only). As for all other file names, "-" may be used to indicate standard output.

- -h Display the program synopsis.
- -t Build a torus rather than a mesh (for gmk\_m2 only).
- -V Print the program version and copyright.

# 7.3.8 gmk\_msh

### **Synopsis**

gmk\_msh [input\_mesh\_file [output\_graph\_file]] options

# Description

The gmk\_msh program builds a graph file from a mesh file. All of the nodes of the mesh are turned into graph vertices, and edges are created between all pairs of vertices that share an element (that is, elements are turned into cliques).

## Options

- -h Display the program synopsis.
- -V Print the program version and copyright.

### 7.3.9 gmtst

# Synopsis

 $\begin{tabular}{ll} $\tt gmtst & [input\_graph\_file & [input\_target\_file & [input\_mapping\_file & [output\_data\_file]]]] options \end{tabular}$ 

### Description

The program gmtst is the graph mapping tester. It outputs some statistics on the given mapping, regarding load balance and inter-processor communication.

The two first statistics lines deal with process mapping statistics, while the following ones deal with communication statistics. The first mapping line gives the number of processors used by the mapping, followed by the number of processors available in the architecture, and the ratio of these two numbers, written between parentheses. The second mapping line gives the minimum, maximum, and average loads of the processors, followed by the variance of the load distribution, and an imbalance ratio equal to the maximum load over the average load. The first communication line gives the minimum and maximum number of neighbors over all blocks of the mapping, followed by the sum of the number of neighbors over all blocks of the mapping, that is the total number of messages that have to be sent to exchange data between all neighboring blocks. The second communication line gives the average dilation of the edges, followed by the sum of all edge dilations. The third communication line gives the average expansion of the edges, followed by the value of function  $f_C$ . The fourth communication line gives the average cut of the edges, followed by the number of cut edges. The fifth communication line shows the ratio of the average expansion over the average dilation; it is smaller than 1 when the mapper succeeds in putting heavily intercommunicating processes closer to each other than it does for lightly communicating processes; it is equal to 1 if all edges have the same weight. The remaining lines form a distance histogram, which shows the amount of communication load that involves processors located at increasing distances.

gmtst allows the testing of cross-architecture mappings. By inputing it a target architecture different from the one that has been used to compute the mapping, but with compatible vertex labels, one can see what the mapping would yield on this new target architecture.

### **Options**

- -h Display the program synopsis.
- -V Print the program version and copyright.

### 7.3.10 gord

### Synopsis

 $gord[input\_graph\_file[output\_ordering\_file[output\_log\_file]]] options$ 

### Description

The gord program is the block sparse matrix graph orderer. It uses an ordering strategy to compute block orderings of sparse matrices represented as

source graphs, whose vertex weights indicate the number of DOFs per node (if this number is non homogeneous) and whose edges are unweighted, in order to minimize fill-in and operation count.

Since its main purpose is to provide orderings that exhibit high concurrency for parallel block factorization, it comprises a nested dissection method [18], but classical [40] and state-of-the-art [1, 48] minimum degree algorithms are implemented as well. Ordering methods are used to define ordering strategies by means of selection, grouping, and condition operators.

For the nested dissection method, vertex separation methods comprise algorithms that directly compute vertex separators, as well as methods that build vertex separators from edge separators, *i.e.* graph bipartitions (all of the graph bipartitioning methods available in the static mapper gmap can be used in this latter case).

The -o option allows the user to define the ordering strategy. The -c option allows the user to set preferences on the behavior of the ordering strategy which is used by default.

When the graphs to order are very large, the same results can be obtained by using the dgord parallel program of the PT-Scotch distribution, which can read centralized graph files too.

### **Options**

Since the program is devoted to experimental studies, it has many optional parameters, used to test various execution modes. Values set by default will give best results in most cases.

## -cflags

Tune the default ordering strategy according to the given preference flags. Some of these flags are antagonistic, while others can be combined. See Section 8.3.1 for more information. The resulting strategy string can be displayed by means of the -vs option.

- b Enforce load balance as much as possible.
- q Privilege quality over speed. This is the default behavior.
- s Privilege speed over quality.
- t Use only safe methods in the strategy.
- -h Display the program synopsis.

#### $-moutput\_mapping\_file$

Write to *output\_mapping\_file* the mapping of graph vertices to column blocks. All of the separators and leaves produced by the nested dissection method are considered as distinct column blocks, which may be in turn split by the ordering methods that are applied to them. Distinct integer numbers are associated with each of the column blocks, such that the number of a block is always greater than the ones of its predecessors in the elimination process, that is, its descendants in the elimination tree. The structure of mapping files is given in section 6.5.

When the geometry of the graph is available, this mapping file may be processed by program gout to display the vertex separators and supervariable amalgamations that have been computed.

#### -ostrat

Apply ordering strategy *strat*. The format of ordering strategies is defined in section 8.3.5.

### -toutput\_tree\_file

Write to *output\_tree\_file* the structure of the separator tree. The data that is written resembles much the one of a mapping file: after a first line that contains the number of lines to follow, there are that many lines of mapping pairs, which associate an integer number with every graph vertex index. This integer number is the number of the column block which is the parent of the column block to which the vertex belongs, or -1 if the column block to which the vertex belongs is a root of the separator tree (there can be several roots, if the graph is disconnected). Combined to the column block mapping data produced by option -m, the tree structure allows one to rebuild the separator tree.

-V Print the program version and copyright.

#### $\neg vverb$

Set verbose mode to *verb*, which may contain several of the following switches.

- s Strategy information. This parameter displays the ordering strategy which will be used by gord.
- t Timing information.

### 7.3.11 gotst

### Synopsis

gotst [input\_graph\_file [input\_ordering\_file [output\_data\_file]]] options

# Description

The program gotst is the ordering tester. It gives some statistics on orderings, including the number of non-zeros and the operation count of the factored matrix, as well as statistics regarding the elimination tree. Since it performs the factorization of the reordered matrix, it can take a very long time and consume a large amount of memory when applied to large graphs.

The first two statistics lines deal with the elimination tree. The first one displays the number of leaves, while the second shows the minimum height of the tree (that is, the length of the shortest path from any leaf to the –or aroot node), its maximum height, its average height, and the variance of the heights with respect to the average. The third line displays the number of non-zero terms in the factored matrix, the amount of index data that is necessary to maintain the block structure of the factored matrix, and the number of operations required to factor the matrix by means of Cholesky factorization.

### Options

- -h Display the program synopsis.
- -V Print the program version and copyright.

### 7.3.12 gout

### **Synopsis**

 $\begin{tabular}{ll} {\tt gout} & [input\_graph\_file & [input\_geometry\_file & [input\_mapping\_file & [output\_visualization\_file]]]] & options \end{tabular}$ 

### Description

The gout program is the graph, matrix, and mapping viewer program. It takes on input a source graph, its geometry file, and optionally a mapping result file, and produces a file suitable for display. At the time being, gout can generate plain and encapsulated PostScript files for the display of adjacency matrix patterns and the display of planar graphs (although tridimensional objects can be displayed by means of isometric projection, the display of tridimensional mappings is not efficient), and OPEN INVENTOR files [41] for the interactive visualization of tridimensional graphs.

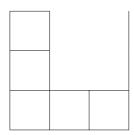
In the case of mapping display, the number of mapping pairs contained in the input mapping file may differ from the number of vertices of the input source graph; only mapping pairs the source labels of which match labels of source graph vertices will be taken into account for display. This feature allows the user to show the result of the mapping of a subgraph drawn on the whole graph, or else to outline the most important aspects of a mapping by restricting the display to a limited portion of the graph. For example, Figure 15.b shows how the result of the mapping of a subgraph of the bidimensional mesh  $M_2(4,4)$  onto the complete graph K(2) can be displayed on the whole  $M_2(4,4)$  graph, and Figure 15.c shows how the display of the same mapping can be restricted to a subgraph of the original graph.

## Options

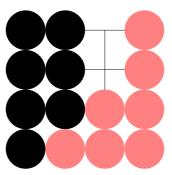
-gparameters

Geometry parameters.

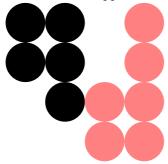
- n Do not read geometry data. This option can be used in conjunction with option -om to avoid reading the geometry file when displaying the pattern of the adjacency matrix associated with the source graph, since geometry data are not needed in this case. If this option is set, the geometry file is not read. However, if an output\_visualization\_file name is given in the command line, dummy input\_geometry\_file and input\_mapping\_file names must be specified so that the file argument count is correct. In this case, use the "-" parameter to take standard input as a dummy geometry input stream. In practice, the -om and -gn options always imply the -mn option.
- r For bidimensional geometry only, rotate geometry data by 90 degrees, counter-clockwise.
- -h Display the program synopsis.
- -mn Do not read mapping data, and display the graph without any mapping information. If this option is set, the mapping file is not read. However, if an output\_visualization\_file name is given in the command line, a dummy input\_mapping\_file name must be specified so that the file argument count is correct. In this case, use the "-" parameter to take standard input as a dummy mapping input stream.



**a.** A subgraph of  $M_2(4,4)$  to be mapped onto K(2).



**b.** Mapping result displayed on the full  $M_2(4,4)$  graph.



**c.** Mapping result displayed on another subgraph of  $M_2(4,4)$ .

Figure 15: PostScript diplay of a single mapping file with different subgraphs of the same source graph. Vertices covered with disks of the same color are mapped onto the same processor.

## $-oformat[\{parameters\}]$

Specify the type of output, with optional parameters within curly braces and separated by commas. The output formats are listed below.

- i Output the graph in SGI's OPEN INVENTOR format, in ASCII mode, suitable for display by the ivview program [41]. The optional parameters are given below.
  - c Color output, using 16 different colors. Opposite of g.
  - g Grey-level output, using 8 different levels. Opposite of c.
  - ${\tt r}$  Remove cut edges. Edges the ends of which are mapped onto different processors are not displayed. Opposite of  ${\tt v}$ .
  - v View cut edges. All graph edges are displayed. Opposite of r.
- m Output the pattern of the adjacency matrix associated with the source graph, in Adobe's PostScript format. The optional parameters are given below.
  - e Encapsulated PostScript output, suitable for LaTeX use with epsf. Opposite of f.
  - f Full-page PostScript output, suitable for direct printing. Opposite of e.
- p Output the graph in Adobe's PostScript format. The optional parameters are given below.

- a Avoid displaying the mapping disks. Opposite of d.
- c Color PostScript output, using 16 different colors. Opposite of g.
- d Display the mapping disks. Opposite of a.
- e Encapsulated PostScript output, suitable for LATEX use with epsf. Opposite of f.
- f Full-page PostScript output, suitable for direct printing. Opposite of e.
- g Grey-level PostScript output. Opposite of c.
- 1 Large clipping. Mapping disks are included in the clipping area computation. Opposite of s.
- r Remove cut edges. Edges the ends of which are mapped onto different processors are not displayed. Opposite of v.
- s Small clipping. Mapping disks are excluded from the clipping area computation. Opposite of 1.
- v View cut edges. All graph edges are displayed. Opposite of  ${\tt r}$ .  ${\tt x=}val$

```
Minimum X relative clipping position (in [0.0;1.0]).
```

X=val

Maximum X relative clipping position (in [0.0;1.0]).

v=vai

Minimum Y relative clipping position (in [0.0;1.0]).

Y = val

Maximum Y relative clipping position (in [0.0;1.0]).

-V Print the program version and copyright.

Default option set is " $-0i\{v\}$ ".

# 7.3.13 gtst

#### **Synopsis**

```
gtst [input_graph_file [output_data_file]] options
```

# Description

The program gtst is the source graph tester. It checks the consistency of the input source graph structure (matching of arcs, number of vertices and edges, etc.), and gives some statistics regarding edge weights, vertex weights, and vertex degrees.

When the graphs to test are very large, the same results can be obtained by using the dgtst parallel program of the PT-Scotch distribution, which can read centralized graph files too.

## Options

- -h Display the program synopsis.
- -V Print the program version and copyright.

#### 7.3.14 mcv

### **Synopsis**

 $mcv [input\_mesh\_file [output\_mesh\_file [output\_geometry\_file]]] options$ 

## Description

The program mcv is the source mesh converter. It takes on input a mesh file of the format specified with the -i option, and outputs its equivalent in the format specified with the -o option, along with its associated geometry file whenever geometrical data is available. At the time being, it only accepts one external input format: the Harwell-Boeing format [10], for square elemental matrices only. The only output format to date is the Scotch source mesh and geometry data format.

### **Options**

-h Display the program synopsis.

## -iformat

Specify the type of input mesh. The available input formats are listed below.

#### b[number]

Harwell-Boeing mesh collection format. Only symmetric elemental matrices are currently supported. Since files in this format can contain several meshes one after another, the optional integer number, starting from 0, indicates which mesh of the file is considered for conversion.

s Scotch source mesh format.

#### -oformat

Specify the output graph format. The available output formats are listed below.

- s Scotch source graph format.
- -V Print the program version and copyright.

Default option set is "-Ib0 -0s".

## 7.3.15 mmk\_\*

### **Synopsis**

```
\label{limits} \begin{tabular}{ll} mmk\_m2 & dimX & [dimY & [output\_mesh\_file]] & options \\ \begin{tabular}{ll} mmk\_m3 & dimX & [dimY & [dimZ & [output\_mesh\_file]]] & options \\ \end{tabular}
```

# Description

The mmk\_\* programs make source meshes.

Program mmk\_m2 outputs the source file of a bidimensional mesh with  $dimX \times dimY$  elements and  $(dimX+1) \times (dimY+1)$  nodes. The element

of coordinates (posX, posY) is labeled  $posY \times dimX + posX$ .

Program mmk\_m3 outputs the source file of a tridimensional mesh with  $dimX \times dimY \times dimZ$  elements and  $(dimX+1) \times (dimY+1) \times (dimZ+1)$  nodes.

# Options

 $-{\tt g} \, output\_geometry\_file$ 

Output mesh geometry to file output\_geometry\_file (for mmk\_m2 only). As for all other file names, "-" may be used to indicate standard output.

- -h Display the program synopsis.
- -V Print the program version and copyright.

#### 7.3.16 mord

## **Synopsis**

 $\verb|mord| input\_mesh\_file| [output\_ordering\_file| [output\_log\_file]]]| options$ 

### Description

The mord program is the block sparse matrix mesh orderer. It uses an ordering strategy to compute block orderings of sparse matrices represented as source meshes, whose node vertex weights indicate the number of DOFs per node (if this number is non homogeneous), in order to minimize fill-in and operation count.

Since its main purpose is to provide orderings that exhibit high concurrency for parallel block factorization, it comprises a nested dissection method [18], but classical [40] and state-of-the-art [1, 48] minimum degree algorithms are implemented as well. Ordering methods are used to define ordering strategies by means of selection, grouping, and condition operators.

The -o option allows the user to define the ordering strategy. The -c option allows the user to set preferences on the behavior of the ordering strategy which is used by default.

#### Options

Since the program is devoted to experimental studies, it has many optional parameters, used to test various execution modes. Values set by default will give best results in most cases.

# -cflags

Tune the default ordering strategy according to the given preference flags. Some of these flags are antagonistic, while others can be combined. See Section 8.3.1 for more information. The resulting strategy string can be displayed by means of the -vs option.

- b Enforce load balance as much as possible.
- ${\tt q}$   $\;\;$  Privilege quality over speed. This is the default behavior.
- s Privilege speed over quality.
- t Use only safe methods in the strategy.

### -h Display the program synopsis.

### $-{\tt m}\, output\_mapping\_file$

Write to *output\_mapping\_file* the mapping of mesh node vertices to column blocks. All of the separators and leaves produced by the nested dissection method are considered as distinct column blocks, which may be in turn split by the ordering methods that are applied to them. Distinct integer numbers are associated with each of the column blocks, such that the number of a block is always greater than the ones of its predecessors in the elimination process, that is, its leaves in the elimination tree. The structure of mapping files is given in section 6.5.

When the coordinates of the node vertices are available, the mapping file may be processed by program gout, along with the graph structure that can be created from the source mesh file by means of the gmk\_msh program, to display the node vertex separators and supervariable amalgamations that have been computed.

#### -ostrai

Apply ordering strategy *strat*. The format of ordering strategies is defined in section 8.3.5.

### $-{\tt t}\,output\_tree\_file$

Write to  $output\_tree\_file$  the structure of the separator tree. The data that is written resembles much the one of a mapping file: after a first line that contains the number of lines to follow, there are that many lines of mapping pairs, which associate an integer number with every node vertex index. This integer number is the number of the column block which is the parent of the column block to which the node vertex belongs, or -1 if the column block to which the node vertex belongs is a root of the separator tree (there can be several roots, if the mesh is disconnected).

Combined to the column block mapping data produced by option -m, the tree structure allows one to rebuild the separator tree.

-V Print the program version and copyright.

### -vverb

Set verbose mode to *verb*, which may contain several of the following switches.

- s Strategy information. This parameter displays the default ordering strategy used by mord.
- t Timing information.

## 7.3.17 mtst

### Synopsis

mtst [input\_mesh\_file [output\_data\_file]] options

# Description

The program mtst is the source mesh tester. It checks the consistency of the input source mesh structure (matching of arcs that link elements to nodes and nodes to elements, number of elements, nodes, and edges, etc.), and gives some statistics regarding element and node weights, edge weights, and element and node degrees.

## Options

- -h Display the program synopsis.
- -V Print the program version and copyright.

# 8 Library

All of the features provided by the programs of the SCOTCH distribution may be directly accessed by calling the appropriate functions of the LIBSCOTCH library, archived in files libscotch.a and libscotcherr.a. These routines belong to six distinct classes:

- source graph and source mesh handling routines, which serve to declare, build, load, save, and check the consistency of source graphs and meshes, along with their geometry data;
- target architecture handling routines, which allow the user to declare, build, load, and save target architectures;
- strategy handling routines, which allow the user to declare and build mapping and ordering strategies;
- mapping routines, which serve to declare, compute, and save mappings of source graphs to target architectures by means of mapping strategies;
- a partitioning-with-overlap routine, which computes a vertex separator that splits a graph into a prescribed number of parts, such that the vertex load of each part and of its neighboring separator vertices are balanced;
- ordering routines, which allow the user to declare, compute, and save orderings of source graphs and meshes;
- error handling routines, which allow the user either to provide his own error servicing routines, or to use the default routines provided in the LIBSCOTCH distribution.

A METIS compatibility library, called libscotchmetis.a, is also available. It allows users who were previously using METIS in their software to take advantage of the efficieny of SCOTCH without having to modify their code. The services provided by this library are described in Section 8.20.

## 8.1 Calling the routines of LIBSCOTCH

#### 8.1.1 Calling from C

All of the C routines of the LIBSCOTCH library are prefixed with "SCOTCH\_". The remainder of the function names is made of the name of the type of object to which the functions apply (e.g. "graph", "mesh", "arch", "map", etc.), followed by the type of action performed on this object: "Init" for the initialization of the object, "Exit" for the freeing of its internal structures, "Load" for loading the object from a stream, and so on.

Typically, functions that return an error code return zero if the function succeeds, and a non-zero value in case of error.

For instance, the SCOTCH\_graphInit and SCOTCH\_graphLoad routines, described in sections 8.6.9 and 8.6.10, respectively, can be called from C by using the following code.

Since "scotch.h" uses several system objects which are declared in "stdio.h", this latter file must be included beforehand in your application code.

Although the "scotch.h" and "ptscotch.h" files may look very similar on your system, never mistake them, and always use the "scotch.h" file as the include file for compiling a program which uses only the sequential routines of the LIBSCOTCH library.

### 8.1.2 Calling from Fortran

The routines of the LIBSCOTCH library can also be called from Fortran. For any C function named SCOTCH\_typeAction() which is documented in this manual, there exists a SCOTCHF TYPEACTION() Fortran counterpart, in which the separating underscore character is replaced by an "F". In most cases, the Fortran routines have exactly the same parameters as the C functions, save for an added trailing INTEGER argument to store the return value yielded by the function when the return type of the C function is not void.

Since all the data structures used in LIBSCOTCH are opaque, equivalent declarations for these structures must be provided in Fortran. These structures must therefore be defined as arrays of DOUBLEPRECISIONS, of sizes given in file scotchf.h, which must be included whenever necessary.

For routines which read or write data using a FILE \* stream in C, the Fortran counterpart uses an INTEGER parameter which is the numer of the Unix file descriptor corresponding to the logical unit from which to read or write. In most Unix implementations of Fortran, standard descriptors 0 for standard input (logical unit 5), 1 for standard output (logical unit 6) and 2 for standard error are opened by default. However, for files which are opened using OPEN statements, an additional function must be used to obtain the number of the Unix file descriptor from the number of the logical unit. This function is called PXFFILENO in the normalized POSIX Fortran API, and files which use it should include the USE IFPOSIX directive whenever necessary. An alternate, non normalized, function also exists in most Unix implementations of Fortran, and is called FNUM.

For instance, the SCOTCH\_graphInit and SCOTCH\_graphLoad routines, described in sections 8.6.9 and 8.6.10, respectively, can be called from Fortran by using the following code.

```
INCLUDE "scotchf.h"

DOUBLEPRECISION GRAFDAT (SCOTCH_GRAPHDIM)

INTEGER RETVAL
...

CALL SCOTCHFGRAPHINIT (GRAFDAT (1), RETVAL)

IF (RETVAL .NE. 0) THEN
...

OPEN (10, FILE='brol.grf')

CALL SCOTCHFGRAPHLOAD (GRAFDAT (1), FNUM (10), 1, 0, RETVAL)

CLOSE (10)

IF (RETVAL .NE. 0) THEN
```

Although the "scotchf.h" and "ptscotchf.h" files may look very similar on your system, never mistake them, and always use the "scotchf.h" file as the include file for compiling a program which uses only the sequential routines of the LIBSCOTCH library.

### 8.1.3 Compiling and linking

The compilation of C or Fortran routines which use routines of the LIBSCOTCH library requires that either "scotch.h" or "scotchf.h" be included, respectively.

The routines of the LIBSCOTCH library are grouped in a library file called libscotch.a. Default error routines that print an error message and exit are provided in library file libscotcherr.a.

Therefore, the linking of applications that make use of the LIBSCOTCH library with standard error handling is carried out by using the following options: "-lscotch -lscotcherr -lm". If you want to handle errors by yourself, you should not link with library file libscotcherr.a, but rather provide a SCOTCH\_errorPrint() routine. Please refer to section 8.18 for more information.

Programs that call both sequential and parallel routines of SCOTCH should use only the parallel versions of the include file and of the library. Please refer to the equivalent section of the PT-SCOTCH user's manual for more information.

# 8.1.4 Dynamic library issues

The advantage of dynamic libraries is that application code may not need to be recompiled when the library is updated. Whether this is true or not depends on the extent of the changes. One of the cases when recompilation is mandatory is when API data structures change: code that statically reserves space for them may be subject to boundary overflow errors when the size of library data structures increase, so that library routines operate on more space than what was statically allocated by the compiler based on the header files of the old version of the library.

In order to alleviate this problem, the LIBSCOTCH proposes a set of routines to dynamically allocate storage space for the opaque API SCOTCH structures. Because these routines return pointers, these SCOTCH\_\*Alloc routines, as well as the SCOTCH\_free routine, are only available in the C interface.

#### 8.1.5 Machine word size issues

Graph indices are represented in Scotch as integer values of type SCOTCH\_Num. By default, this type equates to the int C type, that is, an integer type of size equal to the one of the machine word. However, it can represent any other integer type.

Indeed, the size of the SCOTCH\_Num integer type can be coerced to 32 or 64 bits by using the "-DINTSIZE32" or "-DINTSIZE64" compilation flags, respectively, or else by using the "-DINT=" definition (see Section 9.3 for more information on the setting of these compilation flags).

Consequently, the C interface of Scotch uses two types of integers. Graph-related quantities are passed as SCOTCH\_Nums, while system-related values such as file handles, as well as return values of LIBSCOTCH routines, are always passed as ints.

Because of the variability of library integer type sizes, one must be careful when using the Fortran interface of Scotch, as it does not provide any prototyping information, and consequently cannot produce any warning at link time. In the manual pages of the LIBSCOTCH routines, Fortran prototypes are written using three types of INTEGERs. As for the C interface, the regular INTEGER type is used for system-based values, such as file handles and MPI communicators, as well as for return values of the LIBSCOTCH routines, while the INTEGER\*num type should be used for all graph-related values, in accordance to the size of the SCOTCH\_Num type, as set by the "-DINTSIZEx" compilation flags. Also, the INTEGER\*idx type represents an integer type of a size equivalent to the one of a SCOTCH\_Idx, as set by the "-DIDXSIZEx" compilation flags. Values of this type are used in the Fortran interface to represent arbitrary array indices which can span across the whole address space, and consequently deserve special treatment.

In practice, when SCOTCH is compiled on a 32-bit architecture so as to use 64-bit SCOTCH\_Nums, graph indices should be declared as INTEGER\*8, while error return values should still be declared as plain INTEGER (that is, INTEGER\*4) values. On a 32\_64-bit architecture, irrespective of whether SCOTCH\_Nums are defined as INTEGER\*4 or INTEGER\*8 quantities, the SCOTCH\_Idx type should always be defined as a 64-bit quantity, that is, an INTEGER\*8, because it stores differences between memory addresses, which are represented by 64-bit values. The above is no longer a problem if SCOTCH is compiled such that ints equate 64-bit integers. In this case, there is no need to use any type coercing definition.

The MeTiS v3 compatibility library provided by Scotch can also run on a 64-bit architecture. Yet, if you are willing to use it this way, you will have to replace all int's that are passed to the MeTiS routines by 64-bit integer Scotch\_Num values (even the option configuration values). However, in this case, you will no longer be able to link against the service routines of the genuine MeTiS v3 library, as they are only available as a 32-bit implementation.

### 8.2 Data formats

All of the data used in the LIBSCOTCH interface are of integer type SCOTCH\_Num. To hide the internals of SCOTCH to callers, all of the data structures are opaque, that is, declared within "scotch.h" as dummy arrays of double precision values, for the sake of data alignment. Accessor routines, the names of which end in "Size" and "Data", allow callers to retrieve information from opaque structures.

In all of the following, whenever arrays are defined, passed, and accessed, it is assumed that the first element of these arrays is always labeled as baseval, whether baseval is set to 0 (for C-style arrays) or 1 (for Fortran-style arrays). Scotch internally manages with base values and array pointers so as to process

these arrays accordingly.

#### 8.2.1 Architecture format

Target architecture structures are completely opaque. The only way to describe an architecture is by means of a graph passed to the SCOTCH\_archBuild routine.

### 8.2.2 Graph format

Source graphs are described by means of adjacency lists. The description of a graph requires several SCOTCH\_Num scalars and arrays, as shown in Figures 16 and 17. They have the following meaning:

#### baseval

Base value for all array indexings.

#### vertnbr

Number of vertices in graph.

#### edgenbr

Number of arcs in graph. Since edges are represented by both of their ends, the number of edge data in the graph is twice the number of graph edges.

#### verttab

Array of start indices in edgetab of vertex adjacency sub-arrays.

#### vendtab

Array of after-last indices in edgetab of vertex adjacency sub-arrays. For any vertex i, with baseval  $\leq i < (baseval+vertnbr)$ , vendtab[i] – verttab[i] is the degree of vertex i, and the indices of the neighbors of i are stored in edgetab from edgetab[verttab[i]] to edgetab[vendtab[i] – 1], inclusive.

When all vertex adjacency lists are stored in order in edgetab, it is possible to save memory by not allocating the physical memory for vendtab. In this case, illustrated in Figure 16, verttab is of size vertnbr+1 and vendtab points to verttab+1. This case is referred to as the "compact edge array" case, such that verttab is sorted in ascending order, verttab[baseval] = baseval and verttab[baseval+vertnbr] = (baseval+edgenbr).

#### velotab

Optional array, of size **vertnbr**, holding the integer load associated with every vertex.

### edgetab

Array, of a size equal at least to  $(\max_i(\text{vendtab}[i]) - \text{baseval})$ , holding the adjacency array of every vertex.

### edlotab

Optional array, of a size equal at least to  $(\max_i(\text{vendtab}[i]) - \text{baseval})$ , holding the integer load associated with every arc. Matching arcs should always have identical loads.

Dynamic graphs can be handled elegantly by using the vendtab array. In order to dynamically manage graphs, one just has to allocate verttab, vendtab and edgetab arrays that are large enough to contain all of the expected new vertex and edge data. Original vertices are labeled starting from baseval, leaving free space at

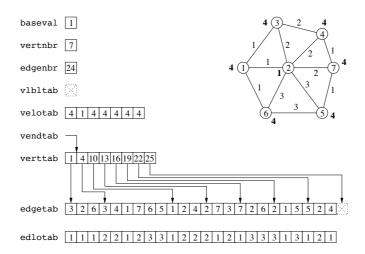


Figure 16: Sample graph and its description by LIBSCOTCH arrays using a compact edge array. Numbers within vertices are vertex indices, bold numbers close to vertices are vertex loads, and numbers close to edges are edge loads. Since the edge array is compact, verttab is of size vertnbr+1 and vendtab points to verttab+1.

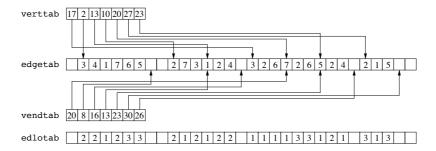


Figure 17: Adjacency structure of the sample graph of Figure 16 with disjoint edge and edge load arrays. Both verttab and vendtab are of size vertnbr. This allows for the handling of dynamic graphs, the structure of which can evolve with time.

the end of the arrays. To remove some vertex i, one just has to replace  $\mathtt{verttab}[i]$  and  $\mathtt{vendtab}[i]$  with the values of  $\mathtt{verttab}[\mathtt{vertnbr-1}]$  and  $\mathtt{vendtab}[\mathtt{vertnbr-1}]$ , respectively, and browse the adjacencies of all neighbors of former vertex  $\mathtt{vertnbr-1}$  such that all ( $\mathtt{vertnbr-1}$ ) indices are turned into is. Then,  $\mathtt{vertnbr}$  must be decremented, and  $\mathtt{SCOTCH\_graphBuild}()$  must be called to account for the change of topology. If a graph building routine such as  $\mathtt{SCOTCH\_graphLoad}()$  or  $\mathtt{SCOTCH\_graphBuild}()$  had already been called on the  $\mathtt{SCOTCH\_graphLoad}()$  or  $\mathtt{SCOTCH\_graphFree}()$  has to be called first in order to free the internal structures associated with the older version of the graph, else these data would be lost, which would result in memory leakage.

To add a new vertex, one has to fill verttab[vertnbr-1] and vendtab[vertnbr-1] with the starting and end indices of the adjacency sub-array of the new vertex. Then, the adjacencies of its neighbor vertices must also be updated to account for it. If free space had been reserved at the end of each of the neighbors, one just has to increment the vendtab[i] values of every neighbor i, and add the index of the new vertex at the end of the adjacency sub-array. If the sub-array cannot be extended, then it has to be copied elsewhere in the edge array, and both verttab[i] and vendtab[i] must be updated accordingly. With simple housekeeping of free areas of the edge array, dynamic arrays can be updated with as little data movement as possible.

### 8.2.3 Mesh format

Since meshes are basically bipartite graphs, source meshes are also described by means of adjacency lists. The description of a mesh requires several SCOTCH\_Num scalars and arrays, as shown in Figure 18. They have the following meaning:

#### velmhas

Base value for element indexings.

#### vnodbas

Base value for node indexings. The base value of the underlying graph, baseval, is set as min(velmbas, vnodbas).

# velmnbr

Number of element vertices in mesh.

# vnodnbr

Number of node vertices in mesh. The overall number of vertices in the underlying graph, vertnbr, is set as velmnbr + vnodnbr.

#### edgenbr

Number of arcs in mesh. Since edges are represented by both of their ends, the number of edge data in the mesh is twice the number of edges.

#### verttab

Array of start indices in edgetab of vertex (that is, both elements and nodes) adjacency sub-arrays.

### vendtab

Array of after-last indices in edgetab of vertex adjacency sub-arrays. For any element or node vertex i, with baseval  $\leq i < (\texttt{baseval} + \texttt{vertnbr})$ , vendtab[i] - verttab[i] is the degree of vertex i, and the indices of the neighbors of i are stored in edgetab from edgetab [verttab[i]] to edgetab [vendtab[i]-1], inclusive.

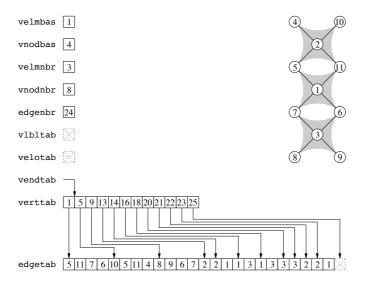


Figure 18: Sample mesh and its description by LIBSCOTCH arrays using a compact edge array. Numbers within vertices are vertex indices. Since the edge array is compact, verttab is of size vertnbr + 1 and vendtab points to verttab + 1.

When all vertex adjacency lists are stored in order in edgetab, it is possible to save memory by not allocating the physical memory for vendtab. In this case, illustrated in Figure 18, verttab is of size vertnbr+1 and vendtab points to verttab+1. This case is referred to as the "compact edge array" case, such that verttab is sorted in ascending order, verttab[baseval] = baseval and verttab[baseval+vertnbr] = (baseval+edgenbr).

### velotab

Array, of size vertnbr, holding the integer load associated with each vertex.

As for graphs, it is possible to handle elegantly dynamic meshes by means of the verttab and vendtab arrays. There is, however, an additional constraint, which is that mesh nodes and elements must be ordered consecutively. The solution to fulfill this constraint in the context of mesh ordering is to keep a set of empty elements (that is, elements which have no node adjacency attached to them) between the element and node arrays. For instance, Figure 19 represents a 4-element mesh with 6 nodes, and such that 4 element vertex slots have been reserved for new elements and nodes. These slots are empty elements for which verttab[i] equals vendtab[i], irrespective of these values, since they will not lead to any memory access in edgetab.

Using this layout of vertices, new nodes and elements can be created by growing the element and node sub-arrays into the empty element sub-array, by both of its sides, without having to re-write the whole mesh structure, as illustrated in Figure 20. Empty elements are transparent to the mesh ordering routines, which base their work on node vertices only. Users who want to update the arrays of a mesh that has already been declared using the SCOTCH\_meshBuild routine must call SCOTCH\_meshExit prior to updating the mesh arrays, and then call SCOTCH\_meshBuild again after the arrays have been updated, so that the SCOTCH\_Mesh structure remains consistent with the new mesh data.

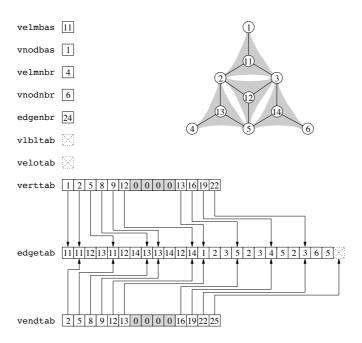


Figure 19: Sample mesh and its description by LIBSCOTCH arrays, with nodes numbered first and elements numbered last. In order to allow for dynamic remeshing, empty elements (in grey) have been inserted between existing node and element vertices.

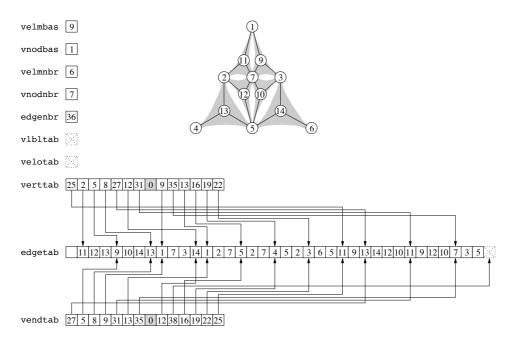


Figure 20: Re-meshing of the mesh of Figure 19. New node vertices have been added at the end of the vertex sub-array, new elements have been added at the beginning of the element sub-array, and vertex base values have been updated accordingly. Node adjacency lists that could not fit in place have been added at the end of the edge array, and some of the freed space has been re-used for new adjacency lists. Element adjacency lists do not require moving in this case, as all of the elements have the name number of nodes.

### 8.2.4 Geometry format

Geometry data is always associated with a graph or a mesh. It is simply made of a single array of double-precision values which represent the coordinates of the vertices of a graph, or of the node vertices of a mesh, in vertex order. The fields of a geometry structure are the following:

#### dimnnbr

Number of dimensions of the graph or of the mesh, which can be 1, 2, or 3.

## geomtab

Array of coordinates. This is an array of double precision values organized as an array of (x), or (x,y), or (x,y,z) tuples, according to dimnnbr. Coordinates that are not used (e.g. the z coordinates for a bidimentional object) are not allocated. Therefore, the x coordinate of some graph vertex i is located at geomtab[(i-baseval)\*dimnnbr+baseval], its y coordinate is located at geomtab[(i-baseval)\*dimnnbr+baseval+1] if dimnnbr  $\geq 2$ , and its z coordinate is located at geomtab[(i-baseval)\*dimnnbr+baseval+2] if dimnnbr = 3. Whenever the geometry is associated with a mesh, only node vertices are considered, so the x coordinate of some mesh node vertex i, with vnodbas  $\leq i$ , is located at geomtab[(i-vnodbas)\*dimnnbr+baseval+1] if dimnnbr  $\geq 2$ , and its z coordinate is located at geomtab[(i-vnodbas)\*dimnnbr+baseval+2] if dimnnbr = 3.

## 8.2.5 Block ordering format

Block orderings associated with graphs and meshes are described by means of block and permutation arrays, made of SCOTCH\_Nums, as shown in Figure 21. In order for all orderings to have the same structure, irrespective of whether they are created from graphs or meshes, all ordering data indices start from baseval, even when they refer to a mesh the node vertices of which are labeled from a vnodbas index such that vnodbas > baseval. Consequently, row indices are related to vertex indices in memory in the following way: row i is associated with vertex i of the SCOTCH\_Graph structure if the ordering was computed from a graph, and with node vertex i+(vnodbas-baseval) of the SCOTCH\_Mesh structure if the ordering was computed from a mesh. Block orderings are made of the following data:

## permtab

Array holding the permutation of the reordered matrix. Thus, if k = permtab[i], then row i of the original matrix is now row k of the reordered matrix, that is, row i is the  $k^{\text{th}}$  pivot.

# peritab

Inverse permutation of the reordered matrix. Thus, if i = peritab[k], then row k of the reordered matrix was row i of the original matrix.

### cblknbr

Number of column blocks (that is, supervariables) in the block ordering.

# rangtab

Array of ranges for the column blocks. Column block c, with baseval  $\leq c < (\text{cblknbr}+\text{baseval})$ , contains columns with indices ranging from rangtab[i] to rangtab[i+1], exclusive, in the reordered matrix. Indices in rangtab

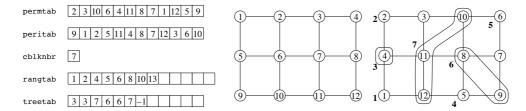


Figure 21: Arrays resulting from the ordering by complete nested dissection of a 4 by 3 grid based from 1. Leftmost grid is the original grid, and righmost grid is the reordered grid, with separators shown and column block indices written in bold.

are based. Therefore, rangtab[baseval] is always equal to baseval, and rangtab[cblknbr+baseval] is always equal to vertnbr+baseval for graphs and to vnodnbr+baseval for meshes. In order to avoid memory errors when column blocks are all single columns, the size of rangtab must always be one more than the number of columns, that is, vertnbr + 1 for graphs and vnodnbr + 1 for meshes.

#### treetab

Array of ascendants of permuted column blocks in the separators tree. treetab[i] is the index of the father of column block i in the separators tree, or -1 if column block i is the root of the separators tree. Whenever separators or leaves of the separators tree are split into subblocks, as the block splitting, minimum fill or minimum degree methods do, all subblocks of the same level are linked to the column block of higher index belonging to the closest separator ancestor. Indices in treetab are based, in the same way as for the other blocking structures. See Figure 21 for a complete example.

# 8.3 Strategy strings

The behavior of the mapping and block ordering routines of the LIBSCOTCH library is parametrized by means of strategy strings, which describe how and when given partitioning or ordering methods should be applied to graphs and subgraphs, or to meshes and submeshes.

#### 8.3.1 Using default strategy strings

While strategy strings can be built by hand, according to the syntax given in the next sections, users who do not have specific needs can take advantage of default strategies already implemented in the LIBSCOTCH, which will yield very good results in most cases. By doing so, they will spare themselves the hassle of updating their strategies to comply to subsequent syntactic changes, and they will benefit from the availability of new partitioning or ordering methods as soon as they are released.

The simplest way to use default strategy strings is to avoid specifying any. By initializing a strategy object, by means of the SCOTCH\_stratInit routine, and by using the initialized strategy object as is, without further parametrization, this object will be filled with a default strategy when passing it as a parameter to the next partitioning or ordering routine to be called. On return, the strategy object will contain a fully specified strategy, tailored for the type of operation which has been requested. Consequently, a fresh strategy object that was used to partition

a graph cannot be used afterward as a default strategy when calling an ordering routine, for instance, as partitioning and ordering strategies are incompatible.

The LIBSCOTCH also provides helper routines which allow users to express their preferences on the kind of strategy that they need. These helper routines, which are of the form SCOTCH\_strat\*Build (see Section 8.15.2 and after), tune default strategy strings according to parameters provided by the user, such as the requested number of parts (used as a hint to select the most efficient partitioning routines), the desired maximum load imbalance ratio, and a set of preference flags. While some of these flags are antagonistic, most of them can be combined, by means of addition or "binary or" operators. These flags are the following. They are grouped by application class.

# Global flags

#### SCOTCH\_STRATDEFAULT

Default behavior. No flags are set.

#### SCOTCH\_STRATBALANCE

Enforce load balance as much as possible.

#### SCOTCH\_STRATQUALITY

Privilege quality over speed.

#### SCOTCH\_STRATSAFETY

Do not use methods that can lead to the occurrence of problematic events, such as floating point exceptions, which could not be properly handled by the calling software.

### SCOTCH\_STRATSPEED

Privilege speed over quality.

# Mapping and partitioning flags

### SCOTCH\_STRATRECURSIVE

Use only recursive bipartitioning methods, and not direct k-way methods. When this flag is not set, any combination of methods can be used, so as to achieve the best result according to other user preferences.

### SCOTCH\_STRATREMAP

Use the strategy for remapping an existing partition.

## Ordering flags

#### SCOTCH\_STRATLEVELMAX

Create at most the prescribed levels of nested dissection separators.

#### SCOTCH\_STRATLEVELMIN

Create at least the prescribed levels of nested dissection separators. When used in conjunction with SCOTCH\_STRATLEVELMAX, the exact number of nested dissection levels will be performed, unless the graph to order is too small.

### SCOTCH\_STRATLEAFSIMPLE

Order nested dissection leaves as cheaply as possible.

### SCOTCH\_STRATSEPASIMPLE

Order nested dissection separators as cheaply as possible.

### 8.3.2 Mapping strategy strings

At the time being, mapping methods only apply to graphs, as there is not yet a mesh mapping tool in the Scotch package. Mapping strategies are made of methods, with optional parameters enclosed between curly braces, and separated by commas, in the form of  $method[\{parameters\}]$ . The currently available mapping methods are the following.

Band method. This method builds a band graph of given width around the current frontier of the k-way partition to which it is applied, and calls a graph mapping strategy to refine the equivalent k-way partition of the band graph. Then, the refined frontier of the band graph is projected back to the current graph. This method was initially presented in [8] in the case of bipartitioning. The parameters of the band bipartitioning method are listed below.

#### bnd=strat

Set the graph mapping strategy to be used on the band graph.

### org=strat

Set the fallback graph mapping strategy to be used on the original graph if the band graph strategy could not be used. The three cases which require the use of this fallback strategy are the following. First, if the separator of the original graph is empty, which makes it impossible to compute a band graph. Second, if any part of the band graph to be built is of the same size as the one of the original graph. Third, if the application of the bnd bipartitioning method to the band graph leads to a situation where any two anchor vertices are placed in the same part.

#### width=val

Set the width of the band graph. All graph vertices that are at a distance less than or equal to *val* from any frontier vertex are kept in the band graph.

Diffusion method. This method, presented in [43] in the case of bipartitioning, flows k kinds of antagonistic liquids from k source vertices, and sets the new frontier as the limit between vertices which contain different kinds of liquids. Because selecting the source vertices is essential to the obtainment of useful results, this method has been hard-coded so that the k source vertices are the k vertices of highest indices, since in the band method these are the anchor vertices which represent all of the removed vertices of each part. Therefore, this method must be used on band graphs only, or on specifically crafted graphs. Applying it to any other graphs is very likely to lead to extremely poor results. The physical analogy of this method loses weight when it is applied to target architectures that are not complete graphs. The parameters of the diffusion mapping method are listed below.

#### dif=rat

Fraction of liquid which is diffused to neighbor vertices at each pass. To achieve convergence, the sum of the dif and rem parameters must be equal to 1, but in order to speed-up the diffusion process, other combinations of higher sum can be tried. In this case, the number of passes must be kept low, to avoid numerical overflows which would make the results useless.

### pass=nbr

Set the number of diffusion sweeps performed by the algorithm. This

number depends on the width of the band graph to which the diffusion method is applied. Useful values range from 30 to 500 according to chosen dif and rem coefficients.

#### rem=rat

Fraction of liquid which remains on vertices at each pass. See above.

 ${\sf f}$  k-way Fiduccia-Mattheyses method. The parameters of the Fiduccia-Mattheyses method are listed below.

### bal=rat

Set the maximum weight imbalance ratio to the given fraction of the subgraph vertex weight. Common values are around 0.01, that is, one percent.

### move=nbr

Maximum number of hill-climbing moves that can be performed before a pass ends. During each of its passes, the Fiduccia-Mattheyses algorithm repeatedly swaps vertices between parts so as to minimize the cost function. A pass completes either when all of the vertices have been moved once, or if too many swaps that do not decrease the value of the cost function have been performed. Setting this value to zero turns the Fiduccia-Mattheyses algorithm into a gradient-like method, which may be used to quickly refine partitions during the uncoarsening phase of the multilevel method.

## pass=nbr

Set the maximum number of optimization passes performed by the algorithm. The Fiduccia-Mattheyses algorithm stops as soon as a pass has not yielded any improvement of the cost function, or when the maximum number of passes has been reached. Value -1 stands for an infinite number of passes, that is, as many as needed by the algorithm to converge.

m Multilevel method. The parameters of the multilevel method are listed below.

#### asc=strat

Set the strategy that is used to refine the mappings obtained at ascending levels of the uncoarsening phase by projection of the mappings computed for coarser graphs. This strategy is not applied to the coarsest graph, for which only the low strategy is used.

#### low=strat

Set the strategy that is used to compute the mapping of the coarsest graph, at the lowest level of the coarsening process.

#### rat=rat

Set the threshold maximum coarsening ratio over which graphs are no longer coarsened. The ratio of any given coarsening cannot be less that 0.5 (case of a perfect matching), and cannot be greater than 1.0. Coarsening stops when either the coarsening ratio is above the maximum coarsening ratio, or the graph has fewer vertices than the minimum number of vertices allowed.

### vert=nbr

Set the threshold under which graphs are no longer coarsened. Coarsening stops when either the coarsening ratio is above the maximum coarsening ratio, or the graph would have fewer vertices than the minimum

number of vertices allowed. When the target architecture is a variable-sized architecture, coarsening stops when the coarsened graph would have less than nbr vertices. When the target architecture is a regular, fixed-size, architecture, coarsening stops when each subdomain would have less than nbr vertices, that is, when the size of the coarsened graph would have less than  $nbr \times \text{domnnbr}$  vertices, where domnnbr is the number of vertices in the target architecture.

r Dual Recursive Bipartitioning mapping algorithm, as defined in section 3.2. The parameters of the DRB mapping method are listed below.

### job=tie

The *tie* flag defines how new jobs are stored in job pools.

- t Tie job pools together. Subjobs are stored in same pool as their parent job. This is the default behavior, as it proves the most efficient in practice.
- u Untie job pools. Subjobs are stored in the next job pool to be pro-

#### map=tie

The *tie* flag defines how results of bipartitioning jobs are propagated to jobs still in pools.

- t Tie both mapping tables together. Results are immediately available to jobs in the same job pool. This is the default behavior.
- u Untie mapping tables. Results are only available to jobs of next pool to be processed.

#### poli=policy

Select jobs according to policy *policy*. Job selection policies define how bipartitioning jobs are ordered within the currently active job pool. Valid policy flags are

- L Most neighbors of higher level.
- 1 Highest level.
- r Random.
- S Most neighbors of smaller size. This is the default behavior.
- s Biggest size.

#### sep=strat

Apply bipartitioning strategy *strat* to each bipartitioning job. A bipartitioning strategy is made of one or several bipartitioning methods, which can be combined by means of strategy operators. Graph bipartitioning strategies are described below.

x Exactifier method, as defined in Section 3.3. This greedy algorithm refines the current mapping so as to reduce load imbalance as much as possible. Since this method does not consider communication minimization, its use should be restricted to cases where achieving load balance is critical and where recursive bipartitioning may fail to achieve it, because of very irregular vertex loads.

# 8.3.3 Graph bipartitioning strategy strings

A graph bipartitioning strategy is made of one or several graph bipartitioning methods, which can be combined by means of strategy operators. Strategy operators are listed below, by increasing precedence.

#### strat1 | strat2

Selection operator. The result of the selection is the best bipartition of the two that are obtained by the separate application of strat1 and strat2 to the current bipartition.

#### $strat1\ strat2$

Combination operator. Strategy strat2 is applied to the bipartition resulting from the application of strategy strat1 to the current bipartition. Typically, the first method used should compute an initial bipartition from scratch, and every following method should use the result of the previous one at its starting point.

#### (strat)

Grouping operator. The strategy enclosed within the parentheses is treated as a single bipartitioning method.

### / cond? strat1[: strat2];

Condition operator. According to the result of the evaluation of condition *cond*, either *strat1* or *strat2* (if it is present) is applied. The condition applies to the characteristics of the current active graph, and can be built from logical and relational operators. Conditional operators are listed below, by increasing precedence.

#### cond1 | cond2

Logical or operator. The result of the condition is true if *cond1* or *cond2* are true, or both.

### cond1&cond2

Logical and operator. The result of the condition is true only if both cond1 and cond2 are true.

#### Lcond

Logical not operator. The result of the condition is true only if *cond* is false.

#### var relop val

Relational operator, where var is a graph variable, val is either a graph variable or a constant of the type of variable var, and relop is one of '<', '=', and '>'. The graph variables are listed below, along with their types.

## deg

The average degree of the current graph. Float.

#### edge

The number of arcs (which is twice the number of edges) of the current graph. Integer.

#### load

The overall vertex load (weight) of the current graph. Integer.

### load0

The vertex load of the first subset of the current bipartition of the current graph. Integer.

### vert

The number of vertices of the current graph. Integer.

## $method[\{parameters\}]$

Bipartitioning method. For bipartitioning methods that can be parametrized,

parameter settings may be provided after the method name. Parameters must be separated by commas, and the whole list be enclosed between curly braces.

The currently available graph bipartitioning methods are the following.

b Band method. This method builds a band graph of given width around the current frontier of the graph to which it is applied, and calls a graph bipartitioning strategy to refine the equivalent bipartition of the band graph. Then, the refined frontier of the band graph is projected back to the current graph. This method, presented in [8], was created to reduce the cost of vertex separator refinement algorithms in a multilevel context, but it improves partition quality too. The same behavior is observed for graph bipartitioning. The parameters of the band bipartitioning method are listed below.

#### bnd=strat

Set the graph bipartitioning strategy to be used on the band graph.

#### org=strat

Set the fallback graph bipartitioning strategy to be used on the original graph if the band graph strategy could not be used. The three cases which require the use of this fallback strategy are the following. First, if the separator of the original graph is empty, which makes it impossible to compute a band graph. Second, if any part of the band graph to be built is of the same size as the one of the original graph. Third, if the application of the bnd bipartitioning method to the band graph leads to a situation where both anchor vertices are placed in the same part.

### width=val

Set the width of the band graph. All graph vertices that are at a distance less than or equal to *val* from any frontier vertex are kept in the band graph.

d Diffusion method. This method, presented in [43], flows two kinds of antagonistic liquids, scotch and anti-scotch, from two source vertices, and sets the new frontier as the limit between vertices which contain scotch and the ones which contain anti-scotch. Because selecting the source vertices is essential to the obtainment of useful results, this method has been hard-coded so that the two source vertices are the two vertices of highest indices, since in the band method these are the anchor vertices which represent all of the removed vertices of each part. Therefore, this method must be used on band graphs only, or on specifically crafted graphs. Applying it to any other graphs is very likely to lead to extremely poor results. The parameters of the diffusion bipartitioning method are listed below.

### dif=rat

Fraction of liquid which is diffused to neighbor vertices at each pass. To achieve convergence, the sum of the dif and rem parameters must be equal to 1, but in order to speed-up the diffusion process, other combinations of higher sum can be tried. In this case, the number of passes must be kept low, to avoid numerical overflows which would make the results useless.

### pass=nbr

Set the number of diffusion sweeps performed by the algorithm. This number depends on the width of the band graph to which the diffusion method is applied. Useful values range from 30 to 500 according to chosen dif and rem coefficients.

#### rem=rat

Fraction of liquid which remains on vertices at each pass. See above.

f Fiduccia-Mattheyses method. The parameters of the Fiduccia-Mattheyses method are listed below.

#### bal=rat

Set the maximum weight imbalance ratio to the given fraction of the subgraph vertex weight. Common values are around 0.01, that is, one percent.

#### move=nbr

Maximum number of hill-climbing moves that can be performed before a pass ends. During each of its passes, the Fiduccia-Mattheyses algorithm repeatedly swaps vertices between the two parts so as to minimize the cost function. A pass completes either when all of the vertices have been moved once, or if too many swaps that do not decrease the value of the cost function have been performed. Setting this value to zero turns the Fiduccia-Mattheyses algorithm into a gradient-like method, which may be used to quickly refine partitions during the uncoarsening phase of the multilevel method.

## pass=nbr

Set the maximum number of optimization passes performed by the algorithm. The Fiduccia-Mattheyses algorithm stops as soon as a pass has not yielded any improvement of the cost function, or when the maximum number of passes has been reached. Value -1 stands for an infinite number of passes, that is, as many as needed by the algorithm to converge.

g Gibbs-Poole-Stockmeyer method. This method has only one parameter.

### pass=nbr

Set the number of sweeps performed by the algorithm.

h Greedy-graph-growing method. This method has only one parameter.

### pass=nbr

Set the number of runs performed by the algorithm.

m Multilevel method. The parameters of the multilevel method are listed below.

#### asc=strat

Set the strategy that is used to refine the partitions obtained at ascending levels of the uncoarsening phase by projection of the bipartitions computed for coarser graphs. This strategy is not applied to the coarsest graph, for which only the low strategy is used.

### low=strat

Set the strategy that is used to compute the partition of the coarsest graph, at the lowest level of the coarsening process.

#### rat=rat

Set the threshold maximum coarsening ratio over which graphs are no longer coarsened. The ratio of any given coarsening cannot be less that

0.5 (case of a perfect matching), and cannot be greater than 1.0. Coarsening stops when either the coarsening ratio is above the maximum coarsening ratio, or the graph has fewer vertices than the minimum number of vertices allowed.

#### vert=nbr

Set the threshold minimum graph size under which graphs are no longer coarsened. Coarsening stops when either the coarsening ratio is above the maximum coarsening ratio, or the coarsened graph would have fewer vertices than the minimum number of vertices allowed.

- x Exactifying method.
- z Zero method. This method moves all of the vertices to the first part. Its main use is to stop the bipartitioning process, if some condition is true, when mapping onto variable-sized architectures (see section 3.2.3).

### 8.3.4 Vertex partitioning strategy strings

Vertex partitioning is a special form of graph partitioning, in which graphs are partitioned into a prescribed number of parts by means of vertex separators rather than of edge separators like in Section 8.3.2. The load balance criterion also differs from common practice: the load to be balanced across all parts comprises not only the load of the vertices which belong to the part, but also the load of all the separator vertices which are their immediate neighbors. Consequently, the load of every separator vertex is accounted for several times, in each of the parts it separates.

Vertex partitioning strategies are made of methods, with optional parameters enclosed between curly braces, and separated by commas, in the form of  $method[\{parameters\}]$ . The currently available mapping methods are the following.

f Fiduccia-Mattheyses method. The parameters of the Fiduccia-Mattheyses method are listed below.

## bal=rat

Set the maximum weight imbalance ratio to the given fraction of the subgraph vertex weight. Common values are around 0.01, that is, one percent.

#### move=nbr

Maximum number of hill-climbing moves that can be performed before a pass ends. During each of its passes, the Fiduccia-Mattheyses algorithm repeatedly moves vertices between parts so as to minimize the cost function. A pass completes either when all of the vertices have been moved once, or if too many swaps that do not decrease the value of the cost function have been performed. Setting this value to zero turns the Fiduccia-Mattheyses algorithm into a gradient-like method, which may be used to quickly refine partitions during the uncoarsening phase of the multilevel method.

### pass=nbr

Set the maximum number of optimization passes performed by the algorithm. The Fiduccia-Mattheyses algorithm stops as soon as a pass has not yielded any improvement of the cost function, or when the maximum

number of passes has been reached. Value -1 stands for an infinite number of passes, that is, as many as needed by the algorithm to converge.

g Gibbs-Poole-Stockmeyer method. This is a k-way version of the original algorithm, in which parts are grown one after the other. Consequently, depending on graph topology, this method is likely to yield disconnected parts, with higher probability as the number of part increases. This method has only one parameter.

## pass=nbr

Set the number of sweeps performed by the algorithm.

h Greedy-graph-growing method. This is a k-way version of the original algorithm, in which parts are grown one after the other. Consequently, depending on graph topology, this method is likely to yield disconnected parts, with higher probability as the number of part increases. This method has only one parameter.

# pass=nbr

Set the number of runs performed by the algorithm.

m Multilevel method. The parameters of the multilevel method are listed below.

#### asc=strat

Set the strategy that is used to refine the partitions obtained at ascending levels of the uncoarsening phase by projection of the bipartitions computed for coarser graphs. This strategy is not applied to the coarsest graph, for which only the low strategy is used.

#### low=strat

Set the strategy that is used to compute the partition of the coarsest graph, at the lowest level of the coarsening process.

#### rat=rat

Set the threshold maximum coarsening ratio over which graphs are no longer coarsened. The ratio of any given coarsening cannot be less that 0.5 (case of a perfect matching), and cannot be greater than 1.0. Coarsening stops when either the coarsening ratio is above the maximum coarsening ratio, or the graph has fewer vertices than the minimum number of vertices allowed.

#### vert=nbr

Set the threshold minimum number of vertices per part under which graphs are no longer coarsened. Coarsening stops when either the coarsening ratio is above the maximum coarsening ratio, or the graph has fewer vertices than the minimum number of vertices allowed.

r Recursive bipartitioning algorithm. The parameters of the recursive bipartitioning method are listed below.

### sep=strat

Apply vertex (node) separation strategy *strat* to each bipartitioning job. A node separation strategy is made of one or several node separation methods, which can be combined by means of strategy operators. Node separation strategies are described in Section 8.3.6.

### 8.3.5 Ordering strategy strings

Ordering strategies are available both for graphs and for meshes. An ordering strategy is made of one or several ordering methods, which can be combined by means of strategy operators. The strategy operators that can be used in ordering strategies are listed below, by increasing precedence.

#### (strat)

Grouping operator. The strategy enclosed within the parentheses is treated as a single ordering method.

### / cond? strat1[: strat2];

Condition operator. According to the result of the evaluation of condition *cond*, either *strat1* or *strat2* (if it is present) is applied. The condition applies to the characteristics of the current node of the separators tree, and can be built from logical and relational operators. Conditional operators are listed below, by increasing precedence.

### $cond1 \mid cond2$

Logical or operator. The result of the condition is true if *cond1* or *cond2* are true, or both.

#### cond1&cond2

Logical and operator. The result of the condition is true only if both *cond1* and *cond2* are true.

### ! cond

Logical not operator. The result of the condition is true only if cond is false.

#### var relop val

Relational operator, where *var* is a node variable, *val* is either a node variable or a constant of the type of variable *var*, and *relop* is one of '<', '=', and '>'. The node variables are listed below, along with their types.

### edge

The number of vertices of the current subgraph. Integer.

#### levl

The level of the subgraph in the separators tree, starting from zero for the initial graph at the root of the tree. Integer.

#### load

The overall vertex load (weight) of the current subgraph. Integer.

# mdeg

The maximum degree of the current subgraph. Integer.

### vert

The number of vertices of the current subgraph. Integer.

## $method[\{parameters\}]$

Graph or mesh ordering method. Available ordering methods are listed below.

The currently available ordering methods are the following.

b Blocking method. This method does not perform ordering by itself, but is used as post-processing to cut into blocks of smaller sizes the separators or large blocks produced by other ordering methods. This is not useful in the context of direct solving methods, because the off-diagonal blocks created by the splitting

of large diagonal blocks are likely to be filled at factoring time. However, in the context of incomplete solving methods such as ILU(k) [30], it can lead to a significant reduction of the required memory space and time, because it helps carving large triangular blocks. The parameters of the blocking method are described below.

#### cmin=size

Set the minimum size of the resulting subblocks, in number of columns. Blocks larger than twice this minimum size are cut into sub-blocks of equal sizes (within one), having a number of columns comprised between size and 2size.

The definition of *size* depends on the size of the graph to order. Large graphs cannot afford very small values, because the number of blocks becomes much too large and limits the acceleration of BLAS 3 routines, while large values do not help reducing enough the complexity of ILU(k) solving.

#### strat = strat

Ordering strategy to be performed. After the ordering strategy is applied, the resulting separators tree is traversed and all of the column blocks that are larger than 2size are split into smaller column blocks, without changing the ordering that has been computed.

c Compression method [2]. The parameters of the compression method are listed below.

#### rat=rat

Set the compression ratio over which graphs and meshes will not be compressed. Useful values range between 0.7 and 0.8.

# $\mathtt{cpr} \texttt{=} strat$

Ordering strategy to use on the compressed graph or mesh if its size is below the compression ratio times the size of the original graph or mesh.

### $\mathtt{unc} = strat$

Ordering strategy to use on the original graph or mesh if the size of the compressed graph or mesh were above the compression ratio times the size of the original graph or mesh.

d Block Halo Approximate Minimum Degree method [48]. The parameters of the Halo Approximate Minimum Degree method are listed below. The Block Halo Approximate Minimum Fill method, described below, is more efficient and should be preferred.

#### cmin=size

Minimum number of columns per column block. All column blocks of width smaller than *size* are amalgamated to their parent column block in the elimination tree, provided that it does not violate the cmax constraint.

### $\mathtt{cmax} = size$

Maximum number of column blocks over which some column block will not amalgamate one of its descendents in the elimination tree. This parameter is mainly designed to provide an upper bound for block size in the context of BLAS3 computations; else, a huge value should be provided.

#### frat = rat

Fill-in ratio over which some column block will not amalgamate one of its descendents in the elimination tree. Typical values range from 0.05 to 0.10.

f Block Halo Approximate Minimum Fill method. The parameters of the Halo Approximate Minimum Fill method are listed below.

#### $\mathtt{cmin} = size$

Minimum number of columns per column block. All column blocks of width smaller than *size* are amalgamated to their parent column block in the elimination tree, provided that it does not violate the cmax constraint.

#### $\mathtt{cmax} = size$

Maximum number of column blocks over which some column block will not amalgamate one of its descendents in the elimination tree. This parameter is mainly designed to provide an upper bound for block size in the context of BLAS3 computations; else, a huge value should be provided.

#### frat = rat

Fill-in ratio over which some column block will not amalgamate one of its descendents in the elimination tree. Typical values range from 0.05 to 0.10.

g Gibbs-Poole-Stockmeyer method. This method is used on separators to reduce the number and extent of extra-diagonal blocks. If the number of extra-diagonal blocks is not relevant, the s method should be preferred. This method has only one parameter.

### pass=nbr

Set the number of sweeps performed by the algorithm.

n Nested dissection method. The parameters of the nested dissection method are given below.

#### ole=strat

Set the ordering strategy that is used on every leaf of the separators tree if the node separation strategy sep has failed to separate it further.

# ose=strat

Set the ordering strategy that is used on every separator of the separators tree.

### sep=strat

Set the node separation strategy that is used on every leaf of the separators tree to make it grow. Node separation strategies are described below, in section 8.3.6.

- s Simple method. Vertices are ordered in their natural order. This method is fast, and should be used to order separators if the number of extra-diagonal blocks is not relevant; else, the g method should be preferred.
- Wesh-to-graph method. Available only for mesh ordering strategies. From the mesh to which this method applies is derived a graph, such that a graph vertex is associated with every node of the mesh, and a clique is created between all vertices which represent nodes that belong to the same element. A graph

ordering strategy is then applied to the derived graph, and this ordering is projected back to the nodes of the mesh. This method is here for evaluation purposes only, as mesh ordering methods are generally more efficient than their graph ordering counterpart.

#### strat = strat

Graph ordering strategy to apply to the associated graph.

### 8.3.6 Node separation strategy strings

A node separation strategy is made of one or several node separation methods, which can be combined by means of strategy operators. Strategy operators are listed below, by increasing precedence.

#### strat1 | strat2

Selection operator. The result of the selection is the best vertex separator of the two that are obtained by the distinct application of strat1 and strat2 to the current separator.

#### strat1 strat2

Combination operator. Strategy *strat2* is applied to the vertex separator resulting from the application of strategy *strat1* to the current separator. Typically, the first method used should compute an initial separation from scratch, and every following method should use the result of the previous one as a starting point.

### (strat)

Grouping operator. The strategy enclosed within the parentheses is treated as a single separation method.

### /cond?strat1[:strat2];

Condition operator. According to the result of the evaluation of condition *cond*, either *strat1* or *strat2* (if it is present) is applied. The condition applies to the characteristics of the current subgraph, and can be built from logical and relational operators. Conditional operators are listed below, by increasing precedence.

#### cond1 | cond2

Logical or operator. The result of the condition is true if *cond1* or *cond2* are true, or both.

### cond1&cond2

Logical and operator. The result of the condition is true only if both cond1 and cond2 are true.

### ! cond

Logical not operator. The result of the condition is true only if *cond* is false.

### var relop val

Relational operator, where var is a graph or node variable, val is either a graph or node variable or a constant of the type of variable var, and relop is one of '<', '=', and '>'. The graph and node variables are listed below, along with their types.

#### levl

The level of the subgraph in the separators tree, starting from zero at the root of the tree. Integer.

#### proc

The number of processors on which the current subgraph is distributed at this level of the separators tree. This variable is available only when calling from routines of the PT-Scotch parallel library. Integer.

#### rank

The rank of the current processor among the group of processors on which the current subgraph is distributed at this level of the separators tree. This variable is available only when calling from routines of the PT-SCOTCH parallel library, for instance to decide which node separation strategy should be used on which processor in a multi-sequential approach. Integer.

#### vert

The number of vertices of the current subgraph. Integer.

The currently available vertex separation methods are the following.

b Band method. Available only for graph separation strategies. This method builds a band graph of given width around the current separator of the graph to which it is applied, and calls a graph separation strategy to refine the equivalent separator of the band graph. Then, the refined separator of the band graph is projected back to the current graph. This method, presented in [8], was created to reduce the cost of separator refinement algorithms in a multilevel context, but it improves partition quality too. The parameters of the band separation method are listed below.

#### bnd=strat

Set the vertex separation strategy to be used on the band graph.

#### org=strat

Set the fallback vertex separation strategy to be used on the original graph if the band graph strategy could not be used. The three cases which require the use of this fallback strategy are the following. First, if the separator of the original graph is empty, which makes it impossible to compute a band graph. Second, if any part of the band graph to be built is of the same size as the one of the original graph. Third, if the application of the bnd vertex separation method to the band graph leads to a situation where both anchor vertices are placed in the same part.

#### width=val

Set the width of the band graph. All graph vertices that are at a distance less than or equal to *val* from any separator vertex are kept in the band graph.

Edge-separation method. Available only for graph separation strategies. This method builds vertex separators from edge separators, by the method proposed by Pothen and Fang [49], which uses a variant of the Hopcroft and Karp algorithm due to Duff [9]. This method is expensive and most often yields poorer results than direct vertex-oriented methods such as the vertex vertex Greedy-graph-growing and the vertex Fiduccia-Mattheyses algorithms. The parameters of the edge-separation method are listed below.

#### bal = val

Set the load imbalance tolerance to *val*, which is a floating-point ratio expressed with respect to the ideal load of the partitions.

#### strat = strat

Set the graph bipartitioning strategy that is used to compute the edge bipartition. The syntax of bipartitioning strategy strings is defined within section 8.3.3, at page 63.

#### width=type

Select the width of the vertex separators built from edge separators. When type is set to  $\mathtt{f}$ , fat vertex separators are built, that hold all of the ends of the edges of the edge cut. When it is set to  $\mathtt{t}$ , a thin vertex separator is built by removing as many vertices as possible from the fat separator.

f Vertex Fiduccia-Mattheyses method. The parameters of the vertex Fiduccia-Mattheyses method are listed below.

#### bal=rat

Set the maximum weight imbalance ratio to the given fraction of the weight of all node vertices. Common values are around 0.01, that is, one percent.

#### move=nbr

Maximum number of hill-climbing moves that can be performed before a pass ends. During each of its passes, the vertex Fiduccia-Mattheyses algorithm repeatedly moves vertices from the separator to any of the two parts, so as to minimize the size of the separator. A pass completes either when all of the vertices have been moved once, or if too many swaps that do not decrease the size of the separator have been performed.

#### pass=nbr

Set the maximum number of optimization passes performed by the algorithm. The vertex Fiduccia-Mattheyses algorithm stops as soon as a pass has not yielded any reduction of the size of the separator, or when the maximum number of passes has been reached. Value -1 stands for an infinite number of passes, that is, as many as needed by the algorithm to converge.

g Gibbs-Poole-Stockmeyer method. Available only for graph separation strategies. This method has only one parameter.

## pass=nbr

Set the number of sweeps performed by the algorithm.

h Vertex greedy-graph-growing method. This method has only one parameter.

# pass=nbr

Set the number of runs performed by the algorithm.

m Vertex multilevel method. The parameters of the vertex multilevel method are listed below.

## asc=strat

Set the strategy that is used to refine the vertex separators obtained at ascending levels of the uncoarsening phase by projection of the separators

computed for coarser graphs or meshes. This strategy is not applied to the coarsest graph or mesh, for which only the low strategy is used.

#### low=strat

Set the strategy that is used to compute the vertex separator of the coarsest graph or mesh, at the lowest level of the coarsening process.

#### rat = rat

Set the threshold maximum coarsening ratio over which graphs or meshes are no longer coarsened. The ratio of any given coarsening cannot be less that 0.5 (case of a perfect matching), and cannot be greater than 1.0. Coarsening stops when either the coarsening ratio is above the maximum coarsening ratio, or the graph or mesh has fewer node vertices than the minimum number of vertices allowed.

## vert=nbr

Set the threshold minimum size under which graphs or meshes are no longer coarsened. Coarsening stops when either the coarsening ratio is above the maximum coarsening ratio, or the graph or mesh has fewer node vertices than the minimum number of vertices allowed.

- t Thinner method. Available only for graph separation strategies. This method quickly eliminates all useless vertices of the current separator. It searches the separator for vertices that have no neighbors in one of the two parts, and moves these vertices to the part they are connected to. This method may be used to refine separators during the uncoarsening phase of the multilevel method, and is faster than a vertex Fiduccia-Mattheyses algorithm with {move =0}.
- Wesh-to-graph method. Available only for mesh separation strategies. From the mesh to which this method applies is derived a graph, such that a graph vertex is associated with every node of the mesh, and a clique is created between all vertices which represent nodes that belong to the same element. A graph separation strategy is then applied to the derived graph, and the separator is projected back to the nodes of the mesh. This method is here for evaluation purposes only, as mesh separation methods are generally more efficient than their graph separation counterpart.

## strat=strat

Graph separation strategy to apply to the associated graph.

- Graph separator viewer. Available only for graph separation strategies. Every call to this method results in the creation, in the current subdirectory, of partial mapping files called "vgraphseparatevw\_output\_nnnnnnn.map", where "nnnnnnn" are increasing decimal numbers, which contain the current state of the two parts and the separator. These mapping files can be used as input by the gout program to produce displays of the evolving shape of the current separator and parts. This is mostly a debugging feature, but it can also have an illustrative interest. While it is only available for graph separation strategies, mesh separation strategies can indirectly use it through the mesh-to-graph separation method.
- z Zero method. This method moves all of the node vertices to the first part, resulting in an empty separator. Its main use is to stop the separation process whenever some condition is true.

# 8.4 Target architecture handling routines

#### 8.4.1 SCOTCH\_archExit

#### **Synopsis**

```
void SCOTCH_archExit (SCOTCH_Arch * archptr)
scotchfarchexit (doubleprecision (*) archdat)
```

# Description

The SCOTCH\_archExit function frees the contents of a SCOTCH\_Arch structure previously initialized by SCOTCH\_archInit. All subsequent calls to SCOTCH\_arch routines other than SCOTCH\_archInit, using this structure as parameter, may yield unpredictable results.

## 8.4.2 SCOTCH\_archInit

## **Synopsis**

#### Description

The SCOTCH\_archInit function initializes a SCOTCH\_Arch structure so as to make it suitable for future operations. It should be the first function to be called upon a SCOTCH\_Arch structure. When the target architecture data is no longer of use, call function SCOTCH\_archExit to free its internal structures.

## Return values

SCOTCH\_archInit returns 0 if the graph structure has been successfully initialized, and 1 else.

## 8.4.3 SCOTCH\_archLoad

# Synopsis

The SCOTCH\_archLoad routine fills the SCOTCH\_Arch structure pointed to by archptr with the source graph description available from stream in the SCOTCH target architecture format (see Section 6.4).

Fortran users must use the PXFFILENO or FNUM functions to obtain the number of the Unix file descriptor fildes associated with the logical unit of the architecture file.

#### Return values

SCOTCH\_archLoad returns 0 if the target architecture structure has been successfully allocated and filled with the data read, and 1 else.

#### 8.4.4 SCOTCH\_archName

## **Synopsis**

#### Description

The SCOTCH\_archName function returns a string containing the name of the architecture pointed to by archptr. Since Fortran routines cannot return string pointers, the scotchfarchname routine takes as second and third parameters a character() array to be filled with the name of the architecture, and the integer size of the array, respectively. If the array is of sufficient size, a trailing nul character is appended to the string to materialize the end of the string (this is the C style of handling character strings).

#### Return values

SCOTCH\_archName returns a non-null character pointer that points to a null-terminated string describing the type of the architecture.

#### 8.4.5 SCOTCH\_archSave

## **Synopsis**

The SCOTCH\_archSave routine saves the contents of the SCOTCH\_Arch structure pointed to by archptr to stream stream, in the SCOTCH target architecture format (see section 6.4).

Fortran users must use the PXFFILENO or FNUM functions to obtain the number of the Unix file descriptor fildes associated with the logical unit of the architecture file.

#### Return values

SCOTCH\_archSave returns 0 if the graph structure has been successfully written to stream, and 1 else.

#### 8.4.6 SCOTCH\_archSize

## Synopsis

```
SCOTCH_Num SCOTCH_archSize (const SCOTCH_Arch * archptr)
scotchfarchsize (doubleprecision (*) archdat,
integer*num archnbr)
```

# Description

The SCOTCH\_archSize function returns the number of nodes of the given target architecture. The Fortran routine has a second parameter, of integer type, which is set on return with the number of nodes of the target architecture.

#### Return values

SCOTCH\_archSize returns the number of nodes of the target architecture.

# 8.5 Target architecture creation routines

## 8.5.1 SCOTCH\_archBuild

# Synopsis

```
int SCOTCH_archBuild (SCOTCH_Arch *
                                            archptr,
                      const SCOTCH_Graph *
                                           grafptr,
                      const SCOTCH_Num
                                            listnbr,
                      const SCOTCH_Num *
                                            listtab,
                      const SCOTCH_Strat * straptr)
scotchfarchbuild (doubleprecision (*) archdat,
                  doubleprecision (*)
                                       grafdat,
                  integer*num
                                       listnbr,
                  integer*num (*)
                                       listtab,
                  doubleprecision (*) stradat,
                  integer
                                       ierr)
```

The SCOTCH\_archBuild routine fills the architecture structure pointed to by archptr with the decomposition-defined target architecture computed by applying the graph bipartitioning strategy pointed to by straptr to the architecture graph pointed to by grafptr.

When listptr is not NULL and listnbr is greater than zero, the decomposition-defined architecture is restricted to the listnbr vertices whose indices are given in the array pointed to by listtab, from listtab[0] to listtab[listnbr - 1]. These indices should have the same base value as the one of the graph pointed to by grafptr, that is, be in the range from 0 to vertnbr -1 if the graph base is 0, and from 1 to vertnbr if the graph base is 1.

Graph bipartitioning strategies are declared by means of the SCOTCH\_strat GraphBipart function, described in page 130. The syntax of bipartitioning strategy strings is defined in section 8.3.2, page 63. Additional information may be obtained from the manual page of amk\_grf, the stand-alone executable that uses function SCOTCH\_archBuild to build decomposition-defined target architecture from source graphs, available at page 34.

#### Return values

SCOTCH\_archBuild returns 0 if the decomposition-defined architecture has been successfully computed, and 1 else.

#### 8.5.2 SCOTCH\_archCmplt

#### **Synopsis**

```
int SCOTCH_archCmplt (SCOTCH_Arch * archptr, const SCOTCH_Num vertnbr) scotchfarchcmplt (doubleprecision (*) archdat, integer *num vertnbr, integer ierr)
```

## Description

The SCOTCH\_archCmplt routine fills the SCOTCH\_Arch structure pointed to by archptr with the description of a complete graph architecture with vertnbr processors, which can be used as input to SCOTCH\_graphMap to perform graph partitioning. A shortcut to this is to use the SCOTCH\_graphPart routine.

#### Return values

SCOTCH\_archCmplt returns 0 if the complete graph target architecture has been successfully built, and 1 else.

## 8.5.3 SCOTCH\_archCmpltw

The SCOTCH\_archCmpltw routine fills the SCOTCH\_Arch structure pointed to by archptr with the description of a weighted complete graph architecture with vertnbr processors. The relative weights of the processors are given in the velotab array. Once the target architecture has been created, it can be used as input to SCOTCH\_graphMap to perform weighted graph partitioning.

## Return values

SCOTCH\_archCmpltw returns 0 if the weighted complete graph target architecture has been successfully built, and 1 else.

#### 8.5.4 SCOTCH\_archHcub

## Synopsis

## Description

The SCOTCH\_archHcub routine fills the SCOTCH\_Arch structure pointed to by archptr with the description of a hypercube graph of dimension hdimval.

#### Return values

 ${\tt SCOTCH\_archHcub}$  returns 0 if the hypercube target architecture has been successfully built, and 1 else.

#### 8.5.5 SCOTCH\_archLtleaf

The SCOTCH\_archLtleaf routine fills the SCOTCH\_Arch structure pointed to by archptr with the description of a labeled, tree-shaped, hierarchical graph architecture with  $\sum_{i=0}^{\text{levlnbr}-1} \text{sizetab}[i]$  processors. Level 0 is the root of the tree. For each level i, with  $0 \le i < \text{levlnbr}$ , sizetab[i] is the number of childs at level (i+1) of each node at level i, and linktab[i] is the cost of communication between processors the first common ancestor of which belongs to this level. See Section 6.4.2, page 26, for an example of this architecture.

#### Return values

SCOTCH\_archLtleaf returns 0 if the labeled tree-leaf target architecture has been successfully built, and 1 else.

## 8.5.6 SCOTCH\_archMesh2D

## **Synopsis**

```
int SCOTCH_archMesh2D (SCOTCH_Arch * archptr, const SCOTCH_Num const SCOTCH_Num ydimval) scotchfarchmesh2d (doubleprecision (*) archdat, integer*num ydimval, integer ydimval, integer ierr)
```

## Description

The SCOTCH\_archMesh2D routine fills the SCOTCH\_Arch structure pointed to by archptr with the description of a 2D mesh architecture with  $xdimval \times ydimval$  processors.

## Return values

SCOTCH\_archMesh2D returns 0 if the 2D mesh target architecture has been successfully built, and 1 else.

## 8.5.7 SCOTCH\_archMesh3D

```
int SCOTCH_archMesh3D (SCOTCH_Arch * archptr, const SCOTCH_Num const SCOTCH_Num ydimval, const SCOTCH_Num zdimval)

scotchfarchmesh3d (doubleprecision (*) archdat, integer*num ydimval, integer*num zdimval, integer*num integer*num integer ierr)
```

The SCOTCH\_archMesh3D routine fills the SCOTCH\_Arch structure pointed to by archptr with the description of a 3D mesh architecture with  $xdimval \times ydimval \times zdimval$  processors.

#### Return values

SCOTCH\_archMesh3D returns 0 if the 3D mesh target architecture has been successfully built, and 1 else.

#### 8.5.8 SCOTCH\_archTleaf

# Synopsis

```
int SCOTCH_archTleaf (SCOTCH_Arch *
                                         archptr,
                     const SCOTCH_Num
                                         levlnbr,
                     const SCOTCH_Num *
                                         sizetab,
                     const SCOTCH_Num * linktab)
scotchfarchtleaf (doubleprecision (*) archdat,
                  integer*num
                                       levlnbr,
                  integer*num (*)
                                       sizetab,
                  integer*num (*)
                                       linktab,
                  integer
                                       ierr)
```

# Description

The SCOTCH\_archTleaf routine fills the SCOTCH\_Arch structure pointed to by archptr with the description of a tree-shaped, hierarchical graph architecture with  $\sum_{i=0}^{\text{levInbr}-1} \text{sizetab}[i]$  processors. Level 0 is the root of the tree. For each level i, with  $0 \leq i < \text{levInbr}$ , sizetab[i] is the number of childs at level (i+1) of each node at level i, and linktab[i] is the cost of communication between processors the first common ancestor of which belongs to this level. See Section 6.4.2, page 26, for an example of this architecture.

## Return values

SCOTCH\_archTleaf returns 0 if the tree-leaf target architecture has been successfully built, and 1 else.

#### 8.5.9 SCOTCH\_archTorus2D

## Synopsis

## Description

The SCOTCH\_archTorus2D routine fills the SCOTCH\_Arch structure pointed to by archptr with the description of a 2D torus architecture with  $xdimval \times ydimval$  processors.

## Return values

SCOTCH\_archTorus2D returns 0 if the 2D torus target architecture has been successfully built, and 1 else.

#### 8.5.10 SCOTCH\_archTorus3D

## Synopsis

```
int SCOTCH_archTorus3D (SCOTCH_Arch *
                                          archptr,
                       const SCOTCH_Num xdimval,
                       const SCOTCH_Num ydimval,
                       const SCOTCH_Num
                                         zdimval)
scotchfarchtorus3d (doubleprecision (*)
                                         archdat,
                    integer*num
                                         xdimval,
                    integer*num
                                         ydimval,
                    integer*num
                                         zdimval,
                    integer
                                         ierr)
```

## Description

The SCOTCH\_archTorus3D routine fills the SCOTCH\_Arch structure pointed to by archptr with the description of a 3D torus architecture with  $xdimval \times ydimval \times zdimval$  processors.

## Return values

SCOTCH\_archTorus3D returns 0 if the 3D torus target architecture has been successfully built, and 1 else.

# 8.6 Graph handling routines

## 8.6.1 SCOTCH\_graphAlloc

#### Synopsis

```
SCOTCH_Graph * SCOTCH_graphAlloc (void)
```

# Description

The SCOTCH\_graphAlloc function allocates a memory area of a size sufficient to store a SCOTCH\_Graph structure. It is the user's responsibility to free this memory when it is no longer needed, using the SCOTCH\_memFree routine. The allocated space must be initialized before use, by means of the SCOTCH\_graph Init routine.

#### Return values

SCOTCH\_graphAlloc returns the pointer to the memory area if it has been successfully allocated, and NULL else.

## 8.6.2 SCOTCH\_graphBase

# Synopsis

# Description

The SCOTCH\_graphBase routine sets the base of all graph indices according to the given base value, and returns the old base value. This routine is a helper for applications that do not handle base values properly.

In Fortan, the old base value is returned in the third parameter of the function call.

#### Return values

SCOTCH\_graphBase returns the old base value.

## 8.6.3 SCOTCH\_graphBuild

```
int SCOTCH_graphBuild (SCOTCH_Graph *
                                            grafptr,
                       const SCOTCH_Num
                                            baseval,
                       const SCOTCH_Num
                                            vertnbr,
                       const SCOTCH_Num *
                                            verttab.
                       const SCOTCH_Num *
                                            vendtab,
                       const SCOTCH_Num *
                                            velotab,
                       const SCOTCH_Num *
                                            vlbltab,
                       const SCOTCH_Num
                                            edgenbr,
                       const SCOTCH_Num *
                                            edgetab,
                                            edlotab)
                       const SCOTCH_Num *
scotchfgraphbuild (doubleprecision (*)
                                         grafdat,
                   integer*num
                                          baseval,
                   integer*num
                                          vertnbr,
                   integer*num (*)
                                          verttab,
                   integer*num(*)
                                          vendtab,
                   integer*num (*)
                                          velotab,
                   integer*num (*)
                                          vlbltab,
                   integer*num
                                          edgenbr,
                   integer*num (*)
                                          edgetab,
                   integer*num(*)
                                          edlotab,
                   integer
                                          ierr)
```

The SCOTCH\_graphBuild routine fills the source graph structure pointed to by grafptr with all of the data that are passed to it.

baseval is the graph base value for index arrays (typically 0 for structures built from C and 1 for structures built from Fortran). vertnbr is the number of vertices. verttab is the adjacency index array, of size (vertnbr + 1) if the edge array is compact (that is, if vendtab equals verttab + 1 or NULL), or of size vertnbr else. vendtab is the adjacency end index array, of size vertnbr if it is disjoint from verttab. velotab is the vertex load array, of size vertnbr if it exists. vlbltab is the vertex label array, of size vertnbr if it exists. edgenbr is the number of arcs (that is, twice the number of edges). edgetab is the adjacency array, of size at least edgenbr (it can be more if the edge array is not compact). edlotab is the arc load array, of size edgenbr if it exists.

The vendtab, velotab, vlbltab and edlotab arrays are optional, and a NULL pointer can be passed as argument whenever they are not defined. Since, in Fortran, there is no null reference, passing the scotchfgraphbuild routine a reference equal to verttab in the velotab or vlbltab fields makes them be considered as missing arrays. The same holds for edlotab when it is passed a reference equal to edgetab. Setting vendtab to refer to one cell after verttab yields the same result, as it is the exact semantics of a compact vertex array.

To limit memory consumption, SCOTCH\_graphBuild does not copy array data, but instead references them in the SCOTCH\_Graph structure. Therefore, great care should be taken not to modify the contents of the arrays passed to SCOTCH\_graphBuild as long as the graph structure is in use. Every update of the arrays should be preceded by a call to SCOTCH\_graphFree, to free internal graph structures, and eventually followed by a new call to SCOTCH\_

graphBuild to re-build these internal structures so as to be able to use the new graph.

To ensure that inconsistencies in user data do not result in an erroneous behavior of the LIBSCOTCH routines, it is recommended, at least in the development stage, to call the SCOTCH\_graphCheck routine on the newly created SCOTCH\_Graph structure before calling any other LIBSCOTCH routine.

#### Return values

SCOTCH\_graphBuild returns 0 if the graph structure has been successfully set with all of the input data, and 1 else.

## 8.6.4 SCOTCH\_graphCheck

# **Synopsis**

# Description

The SCOTCH\_graphCheck routine checks the consistency of the given SCOTCH\_Graph structure. It can be used in client applications to determine if a graph that has been created from used-generated data by means of the SCOTCH\_graphBuild routine is consistent, prior to calling any other routines of the LIBSCOTCH library.

# Return values

SCOTCH\_graphCheck returns 0 if graph data are consistent, and 1 else.

# 8.6.5 SCOTCH\_graphColor

## Synopsis

```
void SCOTCH_graphColor (const SCOTCH_Graph *
                                              grafptr,
                        SCOTCH_Num *
                                              colotab,
                        SCOTCH_Num *
                                              coloptr,
                        SCOTCH_Num
                                             flagval)
scotchfgraphcolor (doubleprecision (*) grafdat,
                   integer*num (*)
                                        colotab,
                   integer num
                                        colombr,
                   integer num
                                        flagval,
                   integer
                                        ierr)
```

The SCOTCH\_graphColor routine computes a coloring of the graph vertices. The colotab array is filled with color values, and the number of colors found is placed into the integer variable colonbr, pointed to by coloptr.

The computed coloring is not guaranteed to be maximal. Indeed, the only algorithm currently implemented is a variant of Luby's algorithm. Due to the operations of this algorithm, the first colors are likely to have many more representatives than the last colors.

Like for partition arrays, color values are not based: color values range from 0 to (colonbr - 1).

The flag value flagval is currently not used. It may be used in the future to select a coloring method. At the time being, a value of 0 should be provided.

#### Return values

 ${\tt SCOTCH\_graphColor}$  returns 0 if the graph coloring has been successfully computed, and 1 else.

## 8.6.6 SCOTCH\_graphData

## Synopsis

```
void SCOTCH_graphData (const SCOTCH_Graph *
                                             grafptr,
                        SCOTCH_Num *
                                               baseptr,
                        SCOTCH_Num *
                                               vertptr,
                        SCOTCH_Num **
                                               verttab,
                        SCOTCH_Num **
                                               vendtab,
                        SCOTCH_Num **
                                               velotab,
                        SCOTCH_Num **
                                               vlbltab,
                        SCOTCH_Num *
                                               edgeptr,
                        SCOTCH_Num **
                                               edgetab,
                        SCOTCH_Num **
                                               edlotab)
scotchfgraphdata (doubleprecision (*)
                                         grafdat,
                   integer*num (*)
                                         indxtab,
                                         baseval,
                   integer*num
                                         vertnbr,
                   integer*num
                   integer*idx
                                         vertidx,
                   integer*idx
                                         vendidx,
                   integer*idx
                                         veloidx,
                   integer*idx
                                         vlblidx,
                   \verb"integer*" num
                                         edgenbr,
                   integer*idx
                                         edgeidx,
                   integer*num
                                         edloidx)
```

## Description

The SCOTCH\_graphData routine is the dual of the SCOTCH\_graphBuild routine. It is a multiple accessor that returns scalar values and array references.

baseptr is the pointer to a location that will hold the graph base value for index arrays (typically 0 for structures built from C and 1 for structures built

from Fortran). vertptr is the pointer to a location that will hold the number of vertices. verttab is the pointer to a location that will hold the reference to the adjacency index array, of size \*vertptr + 1 if the adjacency array is compact, or of size \*vertptr else. vendtab is the pointer to a location that will hold the reference to the adjacency end index array, and is equal to verttab + 1 if the adjacency array is compact. velotab is the pointer to a location that will hold the reference to the vertex load array, of size \*vertptr. vlbltab is the pointer to a location that will hold the reference to the vertex label array, of size vertnbr. edgeptr is the pointer to a location that will hold the number of arcs (that is, twice the number of edges). edgetab is the pointer to a location that will hold the reference to the adjacency array, of size at least \*edgeptr. edlotab is the pointer to a location that will hold the reference to the arc load array, of size \*edgeptr.

Any of these pointers can be set to NULL on input if the corresponding information is not needed. Else, the reference to a dummy area can be provided, where all unwanted data will be written.

Since there are no pointers in Fortran, a specific mechanism is used to allow users to access graph arrays. The scotchfgraphdata routine is passed an integer array, the first element of which is used as a base address from which all other array indices are computed. Therefore, instead of returning references, the routine returns integers, which represent the starting index of each of the relevant arrays with respect to the base input array, or vertidx, the index of verttab, if they do not exist. For instance, if some base array myarray (1) is passed as parameter indxtab, then the first cell of array verttab will be accessible as myarray (vertidx). In order for this feature to behave properly, the indxtab array must be word-aligned with the graph arrays. This is automatically enforced on most systems, but some care should be taken on systems that allow one to access data that is not word-aligned. On such systems, declaring the array after a dummy doubleprecision array can coerce the compiler into enforcing the proper alignment. Also, on 32\_64 architectures, such indices can be larger than the size of a regular INTEGER. This is why the indices to be returned are defined by means of a specific integer type. See Section 8.1.5 for more information on this issue.

## 8.6.7 SCOTCH\_graphExit

# Synopsis

```
void SCOTCH_graphExit (SCOTCH_Graph * grafptr)
scotchfgraphexit (doubleprecision (*) grafdat)
```

# Description

The SCOTCH\_graphExit function frees the contents of a SCOTCH\_Graph structure previously initialized by SCOTCH\_graphInit. All subsequent calls to SCOTCH\_graph routines other than SCOTCH\_graphInit, using this structure as parameter, may yield unpredictable results.

## 8.6.8 SCOTCH\_graphFree

#### Synopsis

```
void SCOTCH_graphFree (SCOTCH_Graph * grafptr)
scotchfgraphfree (doubleprecision (*) grafdat)
```

## Description

The SCOTCH\_graphFree function frees the graph data of a SCOTCH\_Graph structure previously initialized by SCOTCH\_graphInit, but preserves its internal data structures. This call is equivalent to a call to SCOTCH\_graphExit immediately followed by a call to SCOTCH\_graphInit. Consequently, the given SCOTCH\_Graph structure remains ready for subsequent calls to any routine of the LIBSCOTCH library.

## 8.6.9 SCOTCH\_graphInit

## Synopsis

#### Description

The SCOTCH\_graphInit function initializes a SCOTCH\_Graph structure so as to make it suitable for future operations. It should be the first function to be called upon a SCOTCH\_Graph structure. When the graph data is no longer of use, call function SCOTCH\_graphExit to free its internal structures.

#### Return values

SCOTCH\_graphInit returns 0 if the graph structure has been successfully initialized, and 1 else.

# 8.6.10 SCOTCH\_graphLoad

```
int SCOTCH_graphLoad (SCOTCH_Graph *
                                         grafptr,
                       FILE *
                                         stream,
                       SCOTCH_Num
                                         baseval,
                       SCOTCH_Num
                                         flagval)
scotchfgraphload (doubleprecision (*)
                                           grafdat,
                   integer
                                           fildes,
                   \mathtt{integer} * num
                                           baseval,
                   integer*num
                                           flagval,
                   integer
                                           ierr)
```

The SCOTCH\_graphLoad routine fills the SCOTCH\_Graph structure pointed to by grafptr with the source graph description available from stream in the SCOTCH graph format (see section 6.1).

To ease the handling of source graph files by programs written in C as well as in Fortran, the base value of the graph to read can be set to 0 or 1, by setting the baseval parameter to the proper value. A value of -1 indicates that the graph base should be the same as the one provided in the graph description that is read from stream.

The flagval value is a combination of the following integer values, that may be added or bitwise-ored:

- O Keep vertex and edge weights if they are present in the stream data.
- 1 Remove vertex weights. The graph read will have all of its vertex weights set to one, regardless of what is specified in the stream data.
- 2 Remove edge weights. The graph read will have all of its edge weights set to one, regardless of what is specified in the stream data.

Fortran users must use the PXFFILENO or FNUM functions to obtain the number of the Unix file descriptor fildes associated with the logical unit of the graph file.

#### Return values

SCOTCH\_graphLoad returns 0 if the graph structure has been successfully allocated and filled with the data read, and 1 else.

#### 8.6.11 SCOTCH\_graphSave

## Synopsis

## Description

The SCOTCH\_graphSave routine saves the contents of the SCOTCH\_Graph structure pointed to by grafptr to stream stream, in the SCOTCH graph format (see section 6.1).

Fortran users must use the PXFFILENO or FNUM functions to obtain the number of the Unix file descriptor files associated with the logical unit of the graph file.

#### Return values

SCOTCH\_graphSave returns 0 if the graph structure has been successfully written to stream, and 1 else.

## 8.6.12 SCOTCH\_graphSize

## **Synopsis**

## Description

The SCOTCH\_graphSize routine fills the two areas of type SCOTCH\_Num pointed to by vertptr and edgeptr with the number of vertices and arcs (that is, twice the number of edges) of the given graph pointed to by grafptr, respectively.

Any of these pointers can be set to NULL on input if the corresponding information is not needed. Else, the reference to a dummy area can be provided, where all unwanted data will be written.

This routine is useful to get the size of a graph read by means of the SCOTCH\_graphLoad routine, in order to allocate auxiliary arrays of proper sizes. If the whole structure of the graph is wanted, function SCOTCH\_graphData should be preferred.

## 8.6.13 SCOTCH\_graphStat

```
void SCOTCH_graphStat (const SCOTCH_Graph *
                                              grafptr,
                       SCOTCH_Num *
                                              velominptr,
                       SCOTCH_Num *
                                              velomaxptr,
                       SCOTCH_Num *
                                              velosumptr,
                       double *
                                              veloavgptr,
                       double *
                                              velodltptr,
                       SCOTCH_Num *
                                              degrminptr,
                       SCOTCH_Num *
                                              degrmaxptr,
                       double *
                                              degravgptr,
                       double *
                                              degrdltptr,
                       SCOTCH_Num *
                                              edlominptr,
                       SCOTCH_Num *
                                              edlomaxptr,
                       SCOTCH_Num *
                                              edlosumptr,
                       double *
                                              edloavgptr,
                        double *
                                              edlodltptr)
```

```
scotchfgraphstat (doubleprecision (*)
                                        grafdat,
                  integer*num
                                        velomin,
                  integer*num
                                        velomax,
                                        velosum,
                  integer*num
                  doubleprecision
                                        veloavg,
                  doubleprecision
                                        velodlt,
                  integer*num
                                        degrmin,
                                        degrmax,
                  integer*num
                  doubleprecision
                                        degravg,
                  doubleprecision
                                        degrdlt,
                  integer*num
                                        edlomin,
                  integer*num
                                        edlomax,
                  integer*num
                                        edlosum,
                  doubleprecision
                                        edloavg,
                  doubleprecision
                                        edlodlt)
```

The SCOTCH\_graphStat routine produces some statistics regarding the graph structure pointed to by grafptr. velomin, velomax, velosum, veloavg and velodlt are the minimum vertex load, the maximum vertex load, the sum of all vertex loads, the average vertex load, and the variance of the vertex loads, respectively. degrmin, degrmax, degravg and degrdlt are the minimum vertex degree, the maximum vertex degree, the average vertex degree, and the variance of the vertex degrees, respectively. edlomin, edlomax, edlosum, edloavg and edlodlt are the minimum edge load, the maximum edge load, the sum of all edge loads, the average edge load, and the variance of the edge loads, respectively.

# 8.7 High-level graph partitioning, mapping and clustering routines

The routines presented in this section provide high-level functionalities and free the user from the burden of calling in sequence several of the low-level routines described in the next section.

## 8.7.1 SCOTCH\_graphMap

```
int SCOTCH_graphMap (const SCOTCH_Graph *
                                            grafptr,
                     const SCOTCH_Arch *
                                            archptr,
                     const SCOTCH_Strat *
                                            straptr,
                     SCOTCH_Num *
                                            parttab)
scotchfgraphmap (doubleprecision (*)
                                       grafdat,
                 doubleprecision (*)
                                       archdat,
                 doubleprecision (*)
                                       stradat,
                 integer*num (*)
                                       parttab,
                 integer
                                       ierr)
```

The SCOTCH\_graphMap routine computes a mapping of the source graph structure pointed to by grafptr onto the target architecture pointed to by archptr, using the mapping strategy pointed to by straptr (as defined in Section 8.3.2), and returns the mapping data in the array pointed to by parttab.

The parttab array should have been previously allocated, of a size sufficient to hold as many SCOTCH\_Num integers as there are vertices in the source graph.

On return, every cell of the mapping array holds the number of the target vertex to which the corresponding source vertex is mapped. The numbering of target values is *not* based: target vertices are numbered from 0 to the number of target vertices minus 1. This semantics aims at complying with standards such as MPI, in which process ranks start from 0.

When a variable-sized architecture is used (see Section 6.4.3) and a proper strategy is provided (see Section 8.15.2), the SCOTCH\_graphMap routine can cluster the given graph by means of recursive bipartitioning. In this case, clusters are labeled according to a binary scheme: the part equal to the whole graph is numbered 1, its two bipartitioned descendants are labeled 2 and 3, the two descendants of part 2 are labeled 4 and 5, and so on. More generally, clusters are labeled such that the two descendants of any cluster i that has been split are labeled 2i and 2i + 1.

Classical clustering strategies perform recursive bipartitioning of process graphs until some criterion is met: either parts become smaller than some size threshold, or edge density becomes higher than some ratio, etc. If graph mapping is performed using a variable-sized architecture and a classical mapping strategy, recursive bipartitioning will halt only when the load imbalance criterion allows for one of the bipartitioned parts to be empty (that is, most often, parts contains a single vertex).

## Return values

SCOTCH\_graphMap returns 0 if the mapping of the graph has been successfully computed, and 1 else. In this last case, the parttab array may however have been partially or completely filled, but its contents are not significant.

# 8.7.2 SCOTCH\_graphMapFixed

```
int SCOTCH_graphMapFixed (const SCOTCH_Graph *
                                                 grafptr,
                          const SCOTCH_Arch *
                                                 archptr,
                          const SCOTCH_Strat *
                                                 straptr,
                          SCOTCH_Num *
                                                 parttab)
scotchfgraphmapfixed (doubleprecision (*)
                                            grafdat,
                      doubleprecision (*)
                                            archdat.
                      doubleprecision (*)
                                            stradat,
                      integer*num (*)
                                            parttab,
                      integer
                                            ierr)
```

The SCOTCH\_graphMapFixed routine computes a mapping of the source graph structure pointed to by grafptr onto the target architecture pointed to by archptr, using the mapping strategy pointed to by straptr (as defined in Section 8.3.2), and fills the array pointed to by parttab with the mapping data regarding vertices which have not been pre-assigned by the user.

The parttab array should have been previously allocated, of a size sufficient to hold as many SCOTCH\_Num integers as there are vertices in the source graph. It must also have been filled in advance by the user, with data indicating whether vertices have been already pre-assigned to a fixed position or are to be processed by the routine. In each cell of the parttab array, a value of -1 indicates that the vertex is movable, while a value between 0 and the number of target vertices minus 1 indicates that the vertex has been pre-assigned to the given part.

On return, every cell of the mapping array that contained a -1 will hold the number of the target vertex to which the corresponding source vertex is mapped. The numbering of target values is *not* based: target vertices are numbered from 0 to the number of target vertices minus 1. This semantics aims at complying with standards such as MPI, in which process ranks start from 0.

#### Return values

SCOTCH\_graphMapFixed returns 0 if the mapping of the graph has been successfully computed, and 1 else. In this last case, the parttab array may however have been partially or completely filled, but its contents are not significant.

## 8.7.3 SCOTCH\_graphPart

## Synopsis

```
int SCOTCH_graphPart (const SCOTCH_Graph *
                                             grafptr,
                      const SCOTCH_Num
                                             partnbr,
                      const SCOTCH_Strat *
                                            straptr,
                      SCOTCH_Num *
                                             parttab)
scotchfgraphpart (doubleprecision (*)
                                        grafdat,
                  integer*num
                                        partnbr,
                  doubleprecision (*)
                                        stradat,
                  integer*num (*)
                                        parttab,
                  integer
                                        ierr)
```

## Description

The SCOTCH\_graphPart routine computes an edge-separated partition, into partnbr parts, of the source graph structure pointed to by grafptr, using the graph edge partitioning strategy pointed to by stratptr (as defined in Section 8.3.2), and returns the partition data in the array pointed to by parttab.

The parttab array should have been previously allocated, of a size sufficient to hold as many SCOTCH\_Num integers as there are vertices in the source graph.

On return, every cell of the mapping array holds the number of the target vertex to which the corresponding source vertex is mapped. The numbering of target values is *not* based: target vertices are numbered from 0 to partnbr—1. This semantics aims at complying with standards such as MPI, in which process ranks start from 0.

#### Return values

SCOTCH\_graphPart returns 0 if the graph partition has been successfully computed, and 1 else. In the latter case, the parttab array may however have been partially or completely filled, but its contents are not significant.

## 8.7.4 SCOTCH\_graphPartFixed

#### Synopsis

```
int SCOTCH_graphPartFixed (const SCOTCH_Graph *
                                                  grafptr,
                           const SCOTCH_Num
                                                  partnbr,
                           const SCOTCH_Strat *
                                                  straptr,
                           SCOTCH_Num *
                                                 parttab)
scotchfgraphpartfixed (doubleprecision (*) grafdat,
                       integer*num
                                             partnbr,
                       doubleprecision (*)
                                             stradat,
                       integer*num (*)
                                             parttab,
                       integer
                                             ierr)
```

## Description

The SCOTCH\_graphPartFixed routine computes an edge-separated partition, into partnbr parts, of the source graph structure pointed to by grafptr, using the graph edge partitioning strategy pointed to by stratptr (as defined in Section 8.3.2), and fills the array pointed to by parttab with the partitioning data regarding vertices which have not been pre-assigned by the user.

The parttab array should have been previously allocated, of a size sufficient to hold as many SCOTCH\_Num integers as there are vertices in the source graph. It must also have been filled in advance by the user, with data indicating whether vertices have been already pre-assigned to a fixed position or are to be processed by the routine. In each cell of the parttab array, a value of -1 indicates that the vertex is movable, while a value between 0 and the number of target vertices minus 1 indicates that the vertex has been pre-assigned to the given part.

On return, every cell of the mapping array that contained a -1 will hold the number of the target vertex to which the corresponding source vertex is assigned. The numbering of target values is *not* based: target vertices are numbered from 0 to the number of target vertices minus 1. This semantics aims at complying with standards such as MPI, in which process ranks start from 0.

#### Return values

SCOTCH\_graphPartFixed returns 0 if the graph partition has been successfully computed, and 1 else. In the latter case, the parttab array may however have been partially or completely filled, but its contents are not significant.

#### 8.7.5 SCOTCH\_graphPartOvl

## Synopsis

```
int SCOTCH_graphPartOvl (const SCOTCH_Graph *
                                               grafptr,
                         const SCOTCH_Num
                                               partnbr,
                                               straptr,
                         const SCOTCH_Strat *
                         SCOTCH_Num *
                                               parttab)
scotchfgraphpartovl (doubleprecision (*) grafdat,
                     integer*num
                                           partnbr,
                     doubleprecision (*)
                                           stradat,
                     integer*num (*)
                                           parttab,
                     integer
                                           ierr)
```

## Description

The SCOTCH\_graphPartOvl routine computes an overlapped vertex-separated partition, into partnbr parts, of the source graph structure pointed to by grafptr, using the graph vertex partitioning with overlap strategy pointed to by stratptr (as defined in Section 8.3.4), and returns the partition data in the array pointed to by parttab.

The parttab array should have been previously allocated, of a size sufficient to hold as many SCOTCH\_Num integers as there are vertices in the source graph.

On return, every array cell holds the number of the part to which the corresponding vertex is mapped. Regular parts are numbered from 0 to partnbr-1, and separator vertices are labeled with part number -1.

While SCOTCH\_graphMap and SCOTCH\_graphPart are based on edge partitioning methods, SCOTCH\_graphPartOvl relies on a completely distinct set of routines to compute vertex separators. This is why SCOTCH\_graphPartOvl requires strategy strings of a different kind, created by the SCOTCH\_strat GraphPartOvl\* routines only (see Sections 8.15.5 and 8.15.6).

# Return values

SCOTCH\_graphPartOvl returns 0 if the partition of the graph has been successfully computed, and 1 else. In the latter case, the parttab array may however have been partially or completely filled, but its contents are not significant.

# 8.7.6 SCOTCH\_graphRemap

```
int SCOTCH_graphRemap (const SCOTCH_Graph *
                                              grafptr,
                       const SCOTCH_Arch *
                                              archptr,
                       const SCOTCH_Num *
                                              parotab,
                                              emraval.
                       const double
                       const SCOTCH_Num *
                                              vmlotab,
                       const SCOTCH_Strat *
                                              straptr,
                       SCOTCH_Num *
                                              parttab)
scotchfgraphremap (doubleprecision (*)
                                         grafdat,
                   doubleprecision (*)
                                         archdat,
                   integer*num (*)
                                         parotab,
                   doubleprecision
                                         emraval,
                   integer*num (*)
                                          vmlotab,
                   doubleprecision (*)
                                         stradat,
                   integer*num (*)
                                         parttab,
                   integer
                                         ierr)
```

The SCOTCH\_graphRemap routine computes a remapping of the source graph structure pointed to by grafptr onto the target architecture pointed to by archptr, based on the old partition array pointed to by parotab, using the mapping strategy pointed to by straptr (as defined in Section 8.3.2), and returns the mapping data in the array pointed to by parttab.

The parotab array stores the old partition that is used to compute migration costs. Every cell contains values from 0 to the number of target vertices minus 1, or -1 for vertices that did not belong to the old partition (e.g., vertices newly created by graph adaptation, which can be placed at no cost before their associated data is interpolated).

With every source graph vertex is associated an individual integer migration cost, stored in the vmlotab array. These costs are accounted for in the communication cost function to minimize as multiples of the individual migration cost emraval. Since this value is provided as a floating point number, migration costs can be set as fractions or as non-integer multiples of the cut metric communication costs stored as integer edge loads.

The parttab array should have been previously allocated, of a size sufficient to hold as many SCOTCH\_Num integers as there are vertices in the source graph.

On return, every cell of the mapping array holds the number of the target vertex to which the corresponding source vertex is mapped. The numbering of target values is *not* based: target vertices are numbered from 0 to the number of target vertices minus 1. This semantics aims at complying with standards such as MPI, in which process ranks start from 0.

# Return values

SCOTCH\_graphRemap returns 0 if the mapping of the graph has been successfully computed, and 1 else. In this last case, the parttab array may however have been partially or completely filled, but its contents are not significant.

## 8.7.7 SCOTCH\_graphRemapFixed

## Synopsis

```
int SCOTCH_graphRemapFixed (const SCOTCH_Graph *
                                                   grafptr,
                            const SCOTCH_Arch *
                                                   archptr,
                             const SCOTCH_Num *
                                                   parotab,
                             const double
                                                   emraval,
                             const SCOTCH_Num *
                                                   vmlotab,
                             const SCOTCH_Strat *
                                                   straptr,
                            SCOTCH_Num *
                                                   parttab)
scotchfgraphremapfixed (doubleprecision (*)
                                               grafdat,
                         doubleprecision (*)
                                               archdat,
                         integer*num (*)
                                               parotab,
                         doubleprecision
                                               emraval,
                         integer*num (*)
                                               vmlotab,
                         doubleprecision (*)
                                               stradat,
                         integer*num (*)
                                               parttab,
                         integer
                                               ierr)
```

## Description

The SCOTCH\_graphRemapFixed routine computes a remapping of the source graph structure pointed to by grafptr onto the target architecture pointed to by archptr, based on the old partition array pointed to by parotab, using the mapping strategy pointed to by straptr (as defined in Section 8.3.2), and fills the array pointed to by parttab with the mapping data regarding vertices which have not been pre-assigned by the user.

The parotab array stores the old partition that is used to compute migration costs. Every cell contains values from 0 to the number of target vertices minus 1, or -1 for vertices that did not belong to the old partition (e.g., vertices newly created by graph adaptation, which can be placed at no cost before their associated data is interpolated).

With every source graph vertex is associated an individual integer migration cost, stored in the vmlotab array. These costs are accounted for in the communication cost function to minimize as multiples of the individual migration cost emraval. Since this value is provided as a floating point number, migration costs can be set as fractions or as non-integer multiples of the cut metric communication costs stored as integer edge loads.

The parttab array should have been previously allocated, of a size sufficient to hold as many SCOTCH\_Num integers as there are vertices in the source graph. It must also have been filled in advance by the user, with data indicating whether vertices have been already pre-assigned to a fixed position or are to be processed by the routine. In each cell of the parttab array, a value of -1 indicates that the vertex is movable, while a value between 0 and the number of target vertices minus 1 indicates that the vertex has been pre-assigned to the given part.

On return, every cell of the mapping array that contained a -1 will hold the number of the target vertex to which the corresponding source vertex is

mapped. The numbering of target values is *not* based: target vertices are numbered from 0 to the number of target vertices minus 1. This semantics aims at complying with standards such as MPI, in which process ranks start from 0.

#### Return values

SCOTCH\_graphRemapFixed returns 0 if the mapping of the graph has been successfully computed, and 1 else. In this last case, the parttab array may however have been partially or completely filled, with some -1's removed, but its contents are not significant.

#### 8.7.8 SCOTCH\_graphRepart

#### **Synopsis**

```
int SCOTCH_graphRepart (const SCOTCH_Graph *
                                               grafptr,
                        const SCOTCH_Num
                                               partnbr,
                        const SCOTCH_Num *
                                               parotab,
                        const double
                                               emraval,
                        const SCOTCH_Num *
                                               vmlotab,
                        const SCOTCH_Strat *
                                               straptr,
                        SCOTCH_Num *
                                               parttab)
scotchfgraphrepart (doubleprecision (*)
                                          grafdat,
                    integer*num
                                          partnbr,
                    integer*num (*)
                                          parotab,
                    doubleprecision
                                          emraval,
                    integer*num (*)
                                          vmlotab,
                    doubleprecision (*)
                                          stradat,
                    integer*num (*)
                                          parttab,
                    integer
                                          ierr)
```

#### Description

The SCOTCH\_graphRepart routine computes an edge-separated repartition, into partnbr parts, of the source graph structure pointed to by grafptr, based on the old partition array pointed to by parotab, using the partitioning strategy pointed to by straptr (as defined in Section 8.3.2), and returns the partition data in the array pointed to by parttab.

The parotab array stores the old partition that is used to compute migration costs. Every cell contains values from 0 to the number of target vertices minus 1, or -1 for vertices that did not belong to the old partition (e.g., vertices newly created by graph adaptation, which can be assigned to any part at no cost before their associated data is interpolated).

With every source graph vertex is associated an individual integer migration cost, stored in the vmlotab array. These costs are accounted for in the communication cost function to minimize as multiples of the individual migration cost emraval. Since this value is provided as a floating point number, migration costs can be set as fractions or as non-integer multiples of the cut metric communication costs stored as integer edge loads.

The parttab array should have been previously allocated, of a size sufficient to hold as many SCOTCH\_Num integers as there are vertices in the source graph.

On return, every cell of the mapping array holds the number of the target vertex to which the corresponding source vertex is mapped. The numbering of target values is *not* based: target vertices are numbered from 0 to the number of target vertices minus 1. This semantics aims at complying with standards such as MPI, in which process ranks start from 0.

#### Return values

SCOTCH\_graphRepart returns 0 if the graph partition has been successfully computed, and 1 else. In the latter case, the parttab array may however have been partially or completely filled, but its contents are not significant.

#### 8.7.9 SCOTCH\_graphRepartFixed

#### Synopsis

```
int SCOTCH_graphRepartFixed (const SCOTCH_Graph *
                                                    grafptr,
                             const SCOTCH_Num
                                                    partnbr,
                             const SCOTCH_Num *
                                                    parotab,
                             const double
                                                    emraval,
                             const SCOTCH_Num *
                                                    vmlotab,
                             const SCOTCH_Strat *
                                                    straptr,
                             SCOTCH_Num *
                                                    parttab)
scotchfgraphrepartfixed (doubleprecision (*)
                                               grafdat,
                          integer*num
                                               partnbr,
                          integer*num (*)
                                               parotab,
                         doubleprecision
                                                emraval,
                          integer*num (*)
                                                vmlotab,
                          doubleprecision (*)
                                               stradat,
                          integer*num (*)
                                               parttab,
                          integer
                                                ierr)
```

## Description

The SCOTCH\_graphRepartFixed routine computes an edge-separated repartition, into partnbr parts, of the source graph structure pointed to by grafptr, based on the old partition array pointed to by parotab, using the partitioning strategy pointed to by straptr (as defined in Section 8.3.2), and fills the array pointed to by parttab with the mapping data regarding vertices which have not been pre-assigned by the user.

The parotab array stores the old partition that is used to compute migration costs. Every cell contains values from 0 to the number of target vertices minus 1, or -1 for vertices that did not belong to the old partition (e.g., vertices newly created by graph adaptation, which can be assigned to any part at no cost before their associated data is interpolated).

With every source graph vertex is associated an individual integer migration cost, stored in the vmlotab array. These costs are accounted for in the communication cost function to minimize as multiples of the individual migration

cost emraval. Since this value is provided as a floating point number, migration costs can be set as fractions or as non-integer multiples of the cut metric communication costs stored as integer edge loads.

The parttab array should have been previously allocated, of a size sufficient to hold as many SCOTCH\_Num integers as there are vertices in the source graph. It must also have been filled in advance by the user, with data indicating whether vertices have been already pre-assigned to a fixed position or are to be processed by the routine. In each cell of the parttab array, a value of -1 indicates that the vertex is movable, while a value between 0 and the number of target vertices minus 1 indicates that the vertex has been pre-assigned to the given part.

On return, every cell of the mapping array that contained a -1 will hold the number of the target vertex to which the corresponding source vertex is mapped. The numbering of target values is *not* based: target vertices are numbered from 0 to the number of target vertices minus 1. This semantics aims at complying with standards such as MPI, in which process ranks start from 0.

#### Return values

SCOTCH-graphRepartFixed returns 0 if the graph partition has has been successfully computed, and 1 else. In this last case, the parttab array may however have been partially or completely filled, with some -1's removed, but its contents are not significant.

# 8.8 Low-level graph partitioning, mapping and clustering routines

All of the following routines operate on a SCOTCH\_Mapping structure that contains references to the partition and mapping arrays to be filled during the mapping or remapping process.

#### 8.8.1 SCOTCH\_graphMapCompute

#### Synopsis

#### Description

The SCOTCH\_graphMapCompute routine computes a mapping on the given SCOTCH\_Mapping structure pointed to by mappptr using the mapping strategy pointed to by stratptr.

On return, every cell of the mapping array defined by SCOTCH\_mapInit holds the number of the target vertex to which the corresponding source vertex is mapped. The numbering of target values is *not* based: target vertices are numbered from 0 to the number of target vertices, minus 1.

#### Return values

SCOTCH\_graphMapCompute returns 0 if the mapping has been successfully computed, and 1 else. In this latter case, the mapping array may however have been partially or completely filled, but its contents are not significant.

#### 8.8.2 SCOTCH\_graphMapExit

## **Synopsis**

# Description

The SCOTCH\_graphMapExit function frees the contents of a SCOTCH\_Mapping structure previously initialized by SCOTCH\_graphMapInit. All subsequent calls to SCOTCH\_graphMap\* routines other than SCOTCH\_graphMapInit, using this structure as parameter, may yield unpredictable results.

## 8.8.3 SCOTCH\_graphMapFixedCompute

# Synopsis

## Description

The SCOTCH\_graphMapFixedCompute routine computes a mapping on the given SCOTCH\_Mapping structure pointed to by mappptr using the mapping strategy pointed to by stratptr. The mapping must have been built so that its partition array has been filled in advance by the user, with data indicating whether vertices have been already pre-assigned to a fixed position or are to be processed by the routine. In each cell of the parttab array, a value of -1 indicates that the vertex is movable, while a value between 0 and the number

of target vertices minus 1 indicates that the vertex has been pre-assigned to the given part.

On return, every cell of the mapping array defined by SCOTCH\_mapInit that contained a -1 will hold the number of the target vertex to which the corresponding source vertex is mapped. The numbering of target values is *not* based: target vertices are numbered from 0 to the number of target vertices, minus 1.

#### Return values

SCOTCH\_graphMapFixedCompute returns 0 if the mapping has been successfully computed, and 1 else. In this latter case, the mapping array may however have been partially or completely filled, with some -1's removed, but its contents are not significant.

#### 8.8.4 SCOTCH\_graphMapInit

## Synopsis

```
int SCOTCH_graphMapInit (const SCOTCH_Graph *
                                               grafptr,
                         SCOTCH_Mapping *
                                               mappptr,
                         const SCOTCH_Arch *
                                               archptr,
                         SCOTCH_Num *
                                               parttab)
scotchfgraphmapinit (doubleprecision (*)
                                          grafdat,
                     doubleprecision (*)
                                          mappdat,
                     doubleprecision (*)
                                           archdat,
                     integer*num (*)
                                           parttab,
                     integer
                                           ierr)
```

#### Description

The SCOTCH\_graphMapInit routine fills the mapping structure pointed to by mappptr with all of the data that is passed to it. Thus, all subsequent calls to ordering routines such as SCOTCH\_graphMapCompute, using this mapping structure as parameter, will place mapping results in field parttab.

parttab is the pointer to an array of as many SCOTCH\_Nums as there are vertices in the graph pointed to by grafptr, and which will receive the indices of the vertices of the target architecture pointed to by archptr.

It should be the first function to be called upon a SCOTCH\_Mapping structure. When the mapping structure is no longer of use, call function SCOTCH\_graph MapExit to free its internal structures.

## Return values

 ${\tt SCOTCH\_graphMapInit}$  returns 0 if the mapping structure has been successfully initialized, and 1 else.

## 8.8.5 SCOTCH\_graphMapLoad

The SCOTCH\_graphMapLoad routine fills the SCOTCH\_Mapping structure pointed to by mappptr with the mapping data available in the SCOTCH mapping format (see section 6.5) from stream stream. If the source graph has vertex labels attached to its vertices, mapping indices in the input stream are assumed to be vertex labels as well.

Users willing to have subsequent access to the partition data rather than to fill an opaque SCOTCH\_Mapping structure are invited to use the SCOTCH\_graph TabLoad routine instead.

Fortran users must use the PXFFILENO or FNUM functions to obtain the number of the Unix file descriptor fildes associated with the logical unit of the mapping file.

#### Return values

SCOTCH\_graphMapLoad returns 0 if the mapping structure has been successfully loaded from stream, and 1 else.

## 8.8.6 SCOTCH\_graphMapSave

# Synopsis

## Description

The SCOTCH\_graphMapSave routine saves the contents of the SCOTCH\_Mapping structure pointed to by mappptr to stream stream, in the SCOTCH mapping format (see section 6.5).

Fortran users must use the PXFFILENO or FNUM functions to obtain the number of the Unix file descriptor fildes associated with the logical unit of the mapping file.

#### Return values

SCOTCH\_graphMapSave returns 0 if the mapping structure has been successfully written to stream, and 1 else.

#### 8.8.7 SCOTCH\_graphMapView

#### Synopsis

## Description

The SCOTCH\_mapView routine summarizes statistical information on the mapping pointed to by mappptr (load of target processors, number of neighboring domains, average dilation and expansion, edge cut size, distribution of edge dilations), and prints these results to stream stream.

Fortran users must use the PXFFILENO or FNUM functions to obtain the number of the Unix file descriptor fildes associated with the logical unit of the output data file.

## Return values

SCOTCH\_mapView returns 0 if the data has been successfully written to stream, and 1 else.

# 8.8.8 SCOTCH\_graphRemapCompute

```
int SCOTCH_graphRemapCompute (const SCOTCH_Graph *
                                                    grafptr,
                              SCOTCH_Mapping *
                                                    mappptr,
                              SCOTCH_Mapping *
                                                    mapoptr,
                              const double
                                                    emraval,
                              const SCOTCH_Num *
                                                    vmlotab,
                              const SCOTCH_Strat *
                                                    straptr)
scotchfgraphremapcompute (doubleprecision (*)
                                                grafdat,
                          doubleprecision (*)
                                               mappdat,
                          doubleprecision (*) mapodat,
                          doubleprecision
                                                emraval,
                          integer*num (*)
                                                vmlotab,
                          doubleprecision (*) stradat,
                          integer
                                                ierr)
```

The SCOTCH\_graphRemapCompute routine computes a mapping on the given SCOTCH\_Mapping structure pointed to by mappptr, using the mapping strategy pointed to by stratptr, and accounting for migration costs computed based on the already computed partition pointed to by mappptr. This partition should have been created from the same graph and target architecture as the one pointer to by mappptr.

With every source graph vertex is associated an individual integer migration cost, stored in the vmlotab array. These costs are accounted for in the communication cost function to minimize as multiples of the individual migration cost emraval. Since this value is provided as a floating point number, migration costs can be set as fractions or as non-integer multiples of the cut metric communication costs stored as integer edge loads.

On return, every cell of the new mapping array defined by SCOTCH\_mapInit holds the number of the target vertex to which the corresponding source vertex is mapped. The numbering of target values is *not* based: target vertices are numbered from 0 to the number of target vertices, minus 1.

#### Return values

SCOTCH\_graphRemapCompute returns 0 if the remapping has been successfully computed, and 1 else. In this latter case, the mapping array may however have been partially or completely filled, but its contents are not significant.

## 8.8.9 SCOTCH\_graphRemapFixedCompute

# Synopsis

```
int SCOTCH_graphRemapFixedCompute (const SCOTCH_Graph * grafptr,
                                   SCOTCH_Mapping *
                                                         mappptr,
                                   SCOTCH_Mapping *
                                                         mapoptr,
                                   const double
                                                         emraval,
                                   const SCOTCH_Num *
                                                         vmlotab,
                                   const SCOTCH_Strat *
                                                         straptr)
scotchfgraphremapfixedcompute (doubleprecision (*)
                                                    grafdat,
                               doubleprecision (*)
                                                    mappdat,
                               doubleprecision (*)
                                                     mapodat,
                               doubleprecision
                                                     emraval,
                               integer*num (*)
                                                     vmlotab,
                               doubleprecision (*)
                                                    stradat,
                               integer
                                                     ierr)
```

## Description

The SCOTCH\_graphRemapFixedCompute routine computes a mapping on the given SCOTCH\_Mapping structure pointed to by mappptr, using the mapping strategy pointed to by stratptr, and accounting for migration costs computed based on the already computed partition pointed to by mapoptr. This

partition should have been created from the same graph and target architecture as the one pointer to by mappptr.

The partition array of the mapping pointed to by mappptr must have been filled in advance by the user, with data indicating whether vertices have been already pre-assigned to a fixed position or are to be processed by the routine. A value of -1 indicates that the vertex is movable, while a value between 0 and the number of target vertices minus 1 indicates that the vertex has been pre-assigned to the given part.

With every source graph vertex is associated an individual integer migration cost, stored in the vmlotab array. These costs are accounted for in the communication cost function to minimize as multiples of the individual migration cost emraval. Since this value is provided as a floating point number, migration costs can be set as fractions or as non-integer multiples of the cut metric communication costs stored as integer edge loads.

On return, every cell of the new mapping array defined by SCOTCH\_mapInit that contained a -1 holds the number of the target vertex to which the corresponding source vertex is mapped. The numbering of target values is *not* based: target vertices are numbered from 0 to the number of target vertices, minus 1.

#### Return values

SCOTCH\_graphRemapFixedCompute returns 0 if the remapping has been successfully computed, and 1 else. In this latter case, the mapping array may however have been partially or completely filled, with some -1's removed, but its contents are not significant.

## 8.8.10 SCOTCH\_graphTabLoad

#### Synopsis

# Description

The SCOTCH\_graphTabLoad routine fills the parttab part array pointed to by parttab with the mapping data available in the SCOTCH mapping format (see section 6.5) from stream stream.

This routine allows users to fill plain partition arrays rather than opaque mapping structures, as routine SCOTCH\_graphMapLoad does.

The parttab array should have been previously allocated, of a size sufficient to hold as many SCOTCH\_Num integers as there are vertices in the source graph.

Upon completion, array cells contain the indices of the parts to which vertices belong according to the input mapping stream, or -1 if they were not mentioned in the stream. If the source graph has vertex labels attached to its vertices, mapping indices in the input stream are assumed to be vertex labels as well.

Fortran users must use the PXFFILENO or FNUM functions to obtain the number of the Unix file descriptor fildes associated with the logical unit of the mapping file.

#### Return values

SCOTCH\_graphMapLoad returns 0 if the mapping structure has been successfully loaded from stream, and 1 else.

# 8.9 High-level graph ordering routines

This routine provides high-level functionality and frees the user from the burden of calling in sequence several of the low-level routines described in the next section.

#### 8.9.1 SCOTCH\_graphOrder

## **Synopsis**

```
int SCOTCH_graphOrder (const SCOTCH_Graph * grafptr,
                       const SCOTCH_Strat * straptr,
                       SCOTCH_Num *
                                             permtab,
                       SCOTCH_Num *
                                             peritab,
                       SCOTCH_Num *
                                             cblkptr,
                       SCOTCH_Num *
                                             rangtab,
                       SCOTCH_Num *
                                             treetab)
scotchfgraphorder (doubleprecision (*)
                                         grafdat,
                   doubleprecision (*)
                                         stradat,
                   integer*num (*)
                                         permtab,
                   integer*num (*)
                                         peritab,
                   integer*num
                                         cblknbr,
                   integer*num (*)
                                         rangtab,
                   integer*num (*)
                                         treetab,
                   integer
                                         ierr)
```

#### Description

The SCOTCH\_graphOrder routine computes a block ordering of the unknowns of the symmetric sparse matrix the adjacency structure of which is represented by the source graph structure pointed to by grafptr, using the ordering strategy pointed to by stratptr, and returns ordering data in the scalar pointed to by cblkptr and the four arrays permtab, peritab, rangtab and treetab.

The permtab, peritab, rangtab and treetab arrays should have been previously allocated, of a size sufficient to hold as many SCOTCH\_Num integers as there are vertices in the source graph, plus one in the case of rangtab. Any

of the five output fields can be set to NULL if the corresponding information is not needed. Since, in Fortran, there is no null reference, passing a reference to grafptr in these fields will have the same effect.

On return, permtab holds the direct permutation of the unknowns, that is, vertex i of the original graph has index permtab[i] in the reordered graph, while peritab holds the inverse permutation, that is, vertex i in the reordered graph had index peritab[i] in the original graph. All of these indices are numbered according to the base value of the source graph: permutation indices are numbered from baseval to vertnbr + baseval - 1, that is, from 0 to vertnbr - 1 if the graph base is 0, and from 1 to vertnbr if the graph base is 1.

The three other result fields, \*cblkptr, rangtab and treetab, contain data related to the block structure. \*cblkptr holds the number of column blocks of the produced ordering, and rangtab holds the starting indices of each of the permuted column blocks, in increasing order, so that column block i starts at index rangtab [i] and ends at index (rangtab[i+1]-1), inclusive, in the new ordering. treetab holds the separators tree structure, that is, treetab [i] is the index of the father of column block i in the separators tree, or -1 if column block i is the root of the separators tree. Please refer to Section 8.2.5 for more information.

### Return values

SCOTCH\_graphOrder returns 0 if the ordering of the graph has been successfully computed, and 1 else. In this last case, the rangtab, permtab, and peritab arrays may however have been partially or completely filled, but their contents are not significant.

# 8.10 Low-level graph ordering routines

All of the following routines operate on a SCOTCH\_Ordering structure that contains references to the permutation arrays to be filled during the graph ordering process.

## 8.10.1 SCOTCH\_graphOrderCheck

### Synopsis

# Description

The SCOTCH\_graphOrderCheck routine checks the consistency of the given SCOTCH\_Ordering structure pointed to by ordeptr.

# Return values

SCOTCH\_graphOrderCheck returns 0 if ordering data are consistent, and 1 else.

### 8.10.2 SCOTCH\_graphOrderCompute

### **Synopsis**

## Description

The SCOTCH\_graphOrderCompute routine computes a block ordering of the graph structure pointed to by grafptr, using the ordering strategy pointed to by stratptr, and stores its result in the ordering structure pointed to by ordeptr.

On return, the ordering structure holds a block ordering of the given graph (see section 8.10.5 for a description of the ordering fields).

### Return values

SCOTCH\_graphOrderCompute returns 0 if the ordering has been successfully computed, and 1 else. In this latter case, the ordering arrays may however have been partially or completely filled, but their contents are not significant.

# 8.10.3 SCOTCH\_graphOrderComputeList

## **Synopsis**

```
int SCOTCH_graphOrderComputeList (const SCOTCH_Graph *
                                                        grafptr,
                                  SCOTCH_Ordering *
                                                        ordeptr,
                                  SCOTCH_Num
                                                        listnbr,
                                  SCOTCH_Num *
                                                        listtab,
                                  const SCOTCH_Strat * straptr)
scotchfgraphordercompute (doubleprecision (*)
                                               grafdat,
                          doubleprecision (*)
                                               ordedat,
                          integer*num
                                               listnbr,
                          integer*num (*)
                                               listtab,
                          doubleprecision (*) stradat,
                          integer
                                               ierr)
```

### Description

The SCOTCH\_graphOrderComputeList routine computes a block ordering of a subgraph of the graph structure pointed to by grafptr, using the ordering strategy pointed to by stratptr, and stores its result in the ordering structure pointed to by ordeptr. The induced subgraph is described by means of a

vertex list: listnbr holds the number of vertices to keep in the induced subgraph, the indices of which are given, in any order, in the listtab array.

On return, the ordering structure holds a block ordering of the induced subgraph (see section 8.2.5 for a description of the ordering fields). To compute this ordering, graph ordering methods such as the minimum degree and minimum fill methods will base on the original degree of the induced graph vertices, their non-induced neighbors being considered as halo vertices (see Section 4.4 for more information on halo vertices).

Because an ordering always refers to the full graph, the ordering computed by SCOTCH\_graphOrderComputeList is divided into two distinct parts: the induced graph vertices are ordered by applying to the induced graph the strategy provided by the stratptr parameter, while non-induced vertex are ordered consecutively with the highest available indices. Consequently, the permuted indices of induced vertices range from baseval to (listnbr + baseval - 1), while the permuted indices of the remaining vertices range from (listnbr + baseval) to (vertnbr + baseval - 1), inclusive. The separation tree yielded by SCOTCH\_graphOrderComputeList reflects this property: it is made of two branches, the first one corresponding to the induced subgraph, and the second one to the remaining vertices. Since these two subgraphs are not considered to be connected, both will have their own root, represented by a -1 value in the treetab array of the ordering.

### Return values

SCOTCH\_graphOrderComputeList returns 0 if the ordering has been successfully computed, and 1 else. In this latter case, the ordering arrays may however have been partially or completely filled, but their contents are not significant.

# 8.10.4 SCOTCH\_graphOrderExit

# Synopsis

# Description

The SCOTCH\_graphOrderExit function frees the contents of a SCOTCH\_Ordering structure previously initialized by SCOTCH\_graphOrderInit. All subsequent calls to SCOTCH\_graphOrder\* routines other than SCOTCH\_graphOrderInit, using this structure as parameter, may yield unpredictable results.

### 8.10.5 SCOTCH\_graphOrderInit

```
int SCOTCH_graphOrderInit (const SCOTCH_Graph *
                                                   grafptr,
                           SCOTCH_Ordering *
                                                   ordeptr,
                           SCOTCH_Num *
                                                   permtab,
                           SCOTCH_Num *
                                                   peritab,
                           SCOTCH_Num *
                                                   cblkptr,
                           SCOTCH_Num *
                                                   rangtab,
                           SCOTCH_Num *
                                                   treetab)
scotchfgraphorderinit (doubleprecision (*)
                                              grafdat,
                       doubleprecision (*)
                                              ordedat,
                        integer*num (*)
                                              permtab,
                        integer*num (*)
                                              peritab,
                        integer*num
                                              cblknbr,
                        integer*num (*)
                                              rangtab,
                        integer*num (*)
                                              treetab,
                        integer
                                              ierr)
```

The SCOTCH\_graphOrderInit routine fills the ordering structure pointed to by ordeptr with all of the data that are passed to it. Thus, all subsequent calls to ordering routines such as SCOTCH\_graphOrderCompute, using this ordering structure as parameter, will place ordering results in fields permtab, peritab, \*cblkptr, rangtab or treetab, if they are not set to NULL.

permtab is the ordering permutation array, of size vertnbr, peritab is the inverse ordering permutation array, of size vertnbr, cblkptr is the pointer to a SCOTCH\_Num that will receive the number of produced column blocks, rangtab is the array that holds the column block span information, of size vertnbr+1, and treetab is the array holding the structure of the separators tree, of size vertnbr. See the above manual page of SCOTCH\_graphOrder, as well as section 8.2.5, for an explanation of the semantics of all of these fields.

The SCOTCH\_graphOrderInit routine should be the first function to be called upon a SCOTCH\_Ordering structure for ordering graphs. When the ordering structure is no longer of use, the SCOTCH\_graphOrderExit function must be called, in order to to free its internal structures.

### Return values

SCOTCH\_graphOrderInit returns 0 if the ordering structure has been successfully initialized, and 1 else.

# 8.10.6 SCOTCH\_graphOrderLoad

The SCOTCH\_graphOrderLoad routine fills the SCOTCH\_Ordering structure pointed to by ordeptr with the ordering data available in the SCOTCH ordering format (see section 6.6) from stream stream.

Fortran users must use the PXFFILENO or FNUM functions to obtain the number of the Unix file descriptor fildes associated with the logical unit of the ordering file.

### Return values

SCOTCH\_graphOrderLoad returns 0 if the ordering structure has been successfully loaded from stream, and 1 else.

### 8.10.7 SCOTCH\_graphOrderSave

### **Synopsis**

# Description

The SCOTCH\_graphOrderSave routine saves the contents of the SCOTCH\_Ordering structure pointed to by ordeptr to stream stream, in the SCOTCH ordering format (see section 6.6).

Fortran users must use the PXFFILENO or FNUM functions to obtain the number of the Unix file descriptor fildes associated with the logical unit of the ordering file.

# Return values

 $\texttt{SCOTCH\_graphOrderSave}$  returns 0 if the ordering structure has been successfully written to stream, and 1 else.

### 8.10.8 SCOTCH\_graphOrderSaveMap

The SCOTCH\_graphOrderSaveMap routine saves the block partitioning data associated with the SCOTCH\_Ordering structure pointed to by ordeptr to stream stream, in the SCOTCH mapping format (see section 6.5). A target domain number is associated with every block, such that all node vertices belonging to the same block are shown as belonging to the same target vertex. The resulting mapping file can be used by the gout program (see Section 7.3.12) to produce pictures showing the different separators and blocks.

Fortran users must use the PXFFILENO or FNUM functions to obtain the number of the Unix file descriptor fildes associated with the logical unit of the mapping file.

### Return values

SCOTCH\_graphOrderSaveMap returns 0 if the ordering structure has been successfully written to stream, and 1 else.

### 8.10.9 SCOTCH\_graphOrderSaveTree

# Synopsis

### Description

The SCOTCH\_graphOrderSaveTree routine saves the tree hierarchy information associated with the SCOTCH\_Ordering structure pointed to by ordeptr to stream stream.

The format of the tree output file resembles the one of a mapping or ordering file: it is made up of as many lines as there are vertices in the ordering. Each of these lines holds two integer numbers. The first one is the index or the label of the vertex, and the second one is the index of its parent node in the separators tree, or -1 if the vertex belongs to a root node.

Fortran users must use the PXFFILENO or FNUM functions to obtain the number of the Unix file descriptor fildes associated with the logical unit of the tree mapping file.

### Return values

SCOTCH\_graphOrderSaveTree returns 0 if the separators tree structure has been successfully written to stream, and 1 else.

# 8.11 Mesh handling routines

### 8.11.1 SCOTCH\_meshAlloc

# Synopsis

```
SCOTCH_Mesh * SCOTCH_meshAlloc (void)
```

## Description

The SCOTCH\_meshAlloc function allocates a memory area of a size sufficient to store a SCOTCH\_Mesh structure. It is the user's responsibility to free this memory when it is no longer needed, using the SCOTCH\_memFree routine. The allocated space must be initialized before use, by means of the SCOTCH\_mesh Init routine.

### Return values

SCOTCH\_meshAlloc returns the pointer to the memory area if it has been successfully allocated, and NULL else.

# 8.11.2 SCOTCH\_meshBuild

```
int SCOTCH_meshBuild (SCOTCH_Mesh *
                                            meshptr,
                       const SCOTCH_Num
                                            velmbas,
                       const SCOTCH_Num
                                            vnodbas,
                       {\tt const SCOTCH\_Num}
                                            velmnbr,
                       const SCOTCH_Num
                                            vnodnbr,
                       const SCOTCH_Num *
                                            verttab,
                       const SCOTCH_Num *
                                            vendtab,
                       const SCOTCH_Num *
                                            velotab,
                       const SCOTCH_Num *
                                            vnlotab,
                       const SCOTCH_Num *
                                            vlbltab,
                       const SCOTCH_Num
                                            edgenbr,
                       const SCOTCH_Num *
                                            edgetab)
```

```
scotchfmeshbuild (doubleprecision (*)
                                        meshdat,
                  integer*num
                                        velmbas,
                  integer*num
                                        vnodbas,
                  integer*num
                                        velmnbr.
                  integer*num
                                        vnodnbr,
                  integer*num (*)
                                        verttab,
                  integer*num (*)
                                        vendtab,
                  integer*num (*)
                                        velotab,
                  integer*num (*)
                                        vnlotab,
                  integer*num (*)
                                        vlbltab,
                  integer*num
                                        edgenbr,
                                        edgetab,
                  integer*num (*)
                  integer*num
                                        ierr)
```

The SCOTCH\_meshBuild routine fills the source mesh structure pointed to by meshptr with all of the data that is passed to it.

velmbas and vnodbas are the base values for the element and node vertices, respectively. velmbr and vnodnbr are the number of element and node vertices, respectively, such that either velmbas + velmnbr = vnodnbr or vnodbas + vnodnbr = velmnbr holds, and typically min(velmbas, vnodbas) is 0 for structures built from C and 1 for structures built from Fortran. verttab is the adjacency index array, of size (velmnbr + vnodnbr + 1) if the edge array is compact (that is, if vendtab equals vendtab + 1 or NULL), or of size (velmnbr + vnodnbr1) else. vendtab is the adjacency end index array, of size (velmnbr + vnodnbr) if it is disjoint from verttab. velotab is the element vertex load array, of size velmnbr if it exists. vnlotab is the node vertex load array, of size vnodnbr if it exists. vlbltab is the vertex label array, of size (velmnbr+vnodnbr) if it exists. edgenbr is the number of arcs (that is, twice the number of edges). edgetab is the adjacency array, of size at least edgenbr (it can be more if the edge array is not compact).

The vendtab, velotab, vnlotab and vlbltab arrays are optional, and a NULL pointer can be passed as argument whenever they are not defined. Since, in Fortran, there is no null reference, passing the scotchfmeshbuild routine a reference equal to verttab in the velotab, vnlotab or vlbltab fields makes them be considered as missing arrays. Setting vendtab to refer to one cell after verttab yields the same result, as it is the exact semantics of a compact vertex array.

To limit memory consumption, SCOTCH\_meshBuild does not copy array data, but instead references them in the SCOTCH\_Mesh structure. Therefore, great care should be taken not to modify the contents of the arrays passed to SCOTCH\_meshBuild as long as the mesh structure is in use. Every update of the arrays should be preceded by a call to SCOTCH\_meshExit, to free internal mesh structures, and eventually followed by a new call to SCOTCH\_meshBuild to re-build these internal structures so as to be able to use the new mesh.

To ensure that inconsistencies in user data do not result in an erroneous behavior of the LIBSCOTCH routines, it is recommended, at least in the development

stage, to call the SCOTCH\_meshCheck routine on the newly created SCOTCH\_Mesh structure, prior to any other calls to LIBSCOTCH routines.

### Return values

SCOTCH\_meshBuild returns 0 if the mesh structure has been successfully set with all of the input data, and 1 else.

### 8.11.3 SCOTCH\_meshCheck

# Synopsis

# Description

The SCOTCH\_meshCheck routine checks the consistency of the given SCOTCH\_Mesh structure. It can be used in client applications to determine if a mesh that has been created from used-generated data by means of the SCOTCH\_meshBuild routine is consistent, prior to calling any other routines of the LIBSCOTCH library.

### Return values

SCOTCH\_meshCheck returns 0 if mesh data are consistent, and 1 else.

## 8.11.4 SCOTCH\_meshData

```
void SCOTCH_meshData (const SCOTCH_Mesh *
                                             meshptr,
                       SCOTCH_Num *
                                             vebaptr,
                       SCOTCH_Num *
                                             vnbaptr,
                       SCOTCH_Num *
                                             velmptr,
                       SCOTCH_Num *
                                             vnodptr,
                       SCOTCH_Num **
                                             verttab,
                       SCOTCH_Num **
                                             vendtab,
                       SCOTCH_Num **
                                             velotab,
                       SCOTCH_Num **
                                             vnlotab,
                       SCOTCH_Num **
                                             vlbltab,
                       SCOTCH_Num *
                                             edgeptr,
                       SCOTCH_Num **
                                             edgetab,
                       SCOTCH_Num *
                                             degrptr)
```

```
scotchfmeshdata (doubleprecision (*)
                                        meshdat,
                  integer*num (*)
                                        indxtab,
                  integer*num
                                        velobas,
                  integer*num
                                        vnlobas.
                  integer*num
                                        velmnbr,
                  integer*num
                                        vnodnbr,
                  integer*idx
                                        vertidx,
                  integer*idx
                                        vendidx,
                  integer*idx
                                        veloidx,
                  integer*idx
                                        vnloidx,
                  integer*idx
                                        vlblidx,
                  integer*num
                                        edgenbr,
                  integer*idx
                                        edgeidx,
                  integer*num
                                        degrmax)
```

The SCOTCH\_meshData routine is the dual of the SCOTCH\_meshBuild routine. It is a multiple accessor that returns scalar values and array references.

vebaptr and vnbaptr are pointers to locations that will hold the mesh base value for elements and nodes, respectively (the minimum of these two values is typically 0 for structures built from C and 1 for structures built from Fortran). velmptr and vnodptr are pointers to locations that will hold the number of element and node vertices, respectively. verttab is the pointer to a location that will hold the reference to the adjacency index array, of size (\*velmptr + \*vnodptr + 1) if the adjacency array is compact, or of size (\*velmptr+\*vnodptr) else. vendtab is the pointer to a location that will hold the reference to the adjacency end index array, and is equal to verttab + 1if the adjacency array is compact. velotab and vnlotab are pointers to locations that will hold the reference to the element and node vertex load arrays, of sizes \*velmptr and \*vnodptr, respectively. vlbltab is the pointer to a location that will hold the reference to the vertex label array, of size (\*velmptr + \*vnodptr). edgeptr is the pointer to a location that will hold the number of arcs (that is, twice the number of edges). edgetab is the pointer to a location that will hold the reference to the adjacency array, of size at least edgenbr. degrptr is the pointer to a location that will hold the maximum vertex degree computed across all element and node vertices.

Any of these pointers can be set to NULL on input if the corresponding information is not needed. Else, the reference to a dummy area can be provided, where all unwanted data will be written.

Since there are no pointers in Fortran, a specific mechanism is used to allow users to access mesh arrays. The scotchfmeshdata routine is passed an integer array, the first element of which is used as a base address from which all other array indices are computed. Therefore, instead of returning references, the routine returns integers, which represent the starting index of each of the relevant arrays with respect to the base input array, or vertidx, the index of verttab, if they do not exist. For instance, if some base array myarray (1) is passed as parameter indxtab, then the first cell of array verttab will be accessible as myarray(vertidx). In order for this feature to behave properly, the indxtab array must be word-aligned with the mesh arrays. This is

automatically enforced on most systems, but some care should be taken on systems that allow one to access data that is not word-aligned. On such systems, declaring the array after a dummy doubleprecision array can coerce the compiler into enforcing the proper alignment. Also, on 32\_64 architectures, such indices can be larger than the size of a regular INTEGER. This is why the indices to be returned are defined by means of a specific integer type. See Section 8.1.5 for more information on this issue.

### 8.11.5 SCOTCH\_meshExit

# **Synopsis**

```
void SCOTCH_meshExit (SCOTCH_Mesh * meshptr)
scotchfmeshexit (doubleprecision (*) meshdat)
```

## Description

The SCOTCH\_meshExit function frees the contents of a SCOTCH\_Mesh structure previously initialized by SCOTCH\_meshInit. All subsequent calls to SCOTCH\_mesh\* routines other than SCOTCH\_meshInit, using this structure as parameter, may yield unpredictable results.

### 8.11.6 SCOTCH\_meshGraph

### **Synopsis**

## Description

The SCOTCH\_meshGraph routine builds a graph from a mesh. It creates in the SCOTCH\_Graph structure pointed to by grafptr a graph having as many vertices as there are nodes in the SCOTCH\_Mesh structure pointed to by meshptr, and where there is an edge between any two graph vertices if and only if there exists in the mesh an element containing both of the associated nodes. Consequently, all of the elements of the mesh are turned into cliques in the resulting graph.

In order to save memory space as well as computation time, in the current implementation of SCOTCH\_meshGraph, some mesh arrays are shared with the graph structure. Therefore, one should make sure that the graph must no longer be used after the mesh structure is freed. The graph structure can be freed before or after the mesh structure, but must not be used after the mesh structure is freed.

### Return values

SCOTCH\_meshGraph returns 0 if the graph structure has been successfully allocated and filled, and 1 else.

# 8.11.7 SCOTCH\_meshInit

# **Synopsis**

## Description

The SCOTCH\_meshInit function initializes a SCOTCH\_Mesh structure so as to make it suitable for future operations. It should be the first function to be called upon a SCOTCH\_Mesh structure. When the mesh data is no longer of use, call function SCOTCH\_meshExit to free its internal structures.

### Return values

SCOTCH\_meshInit returns 0 if the mesh structure has been successfully initialized, and 1 else.

### 8.11.8 SCOTCH\_meshLoad

### Synopsis

# Description

The SCOTCH\_meshLoad routine fills the SCOTCH\_Mesh structure pointed to by meshptr with the source mesh description available from stream in the SCOTCH mesh format (see section 6.2).

To ease the handling of source mesh files by programs written in C as well as in Fortran, The base value of the mesh to read can be set to 0 or 1, by setting the baseval parameter to the proper value. A value of -1 indicates that the mesh base should be the same as the one provided in the mesh description that is read from stream.

Fortran users must use the PXFFILENO or FNUM functions to obtain the number of the Unix file descriptor fildes associated with the logical unit of the mesh file.

### Return values

SCOTCH\_meshLoad returns 0 if the mesh structure has been successfully allocated and filled with the data read, and 1 else.

### 8.11.9 SCOTCH\_meshSave

### Synopsis

# Description

The SCOTCH\_meshSave routine saves the contents of the SCOTCH\_Mesh structure pointed to by meshptr to stream stream, in the SCOTCH mesh format (see section 6.2).

Fortran users must use the PXFFILENO or FNUM functions to obtain the number of the Unix file descriptor fildes associated with the logical unit of the mesh file.

## Return values

SCOTCH\_meshSave returns 0 if the mesh structure has been successfully written to stream, and 1 else.

# 8.11.10 SCOTCH\_meshSize

# Synopsis

# Description

The SCOTCH\_meshSize routine fills the three areas of type SCOTCH\_Num pointed to by velmptr, vnodptr and edgeptr with the number of element vertices, node vertices and arcs (that is, twice the number of edges) of the given mesh pointed to by meshptr, respectively.

Any of these pointers can be set to NULL on input if the corresponding information is not needed. Else, the reference to a dummy area can be provided, where all unwanted data will be written.

This routine is useful to get the size of a mesh read by means of the SCOTCH\_meshLoad routine, in order to allocate auxiliary arrays of proper sizes. If the whole structure of the mesh is wanted, function SCOTCH\_meshData should be preferred.

### 8.11.11 SCOTCH\_meshStat

### **Synopsis**

```
void SCOTCH_meshStat (const SCOTCH_Mesh *
                                             meshptr,
                       SCOTCH_Num *
                                             vnlominptr,
                       SCOTCH_Num *
                                             vnlomaxptr,
                       SCOTCH_Num *
                                             vnlosumptr,
                       double *
                                             vnloavgptr,
                       double *
                                             vnlodltptr,
                       SCOTCH_Num *
                                             edegminptr,
                       SCOTCH_Num *
                                             edegmaxptr,
                       double *
                                             edegavgptr,
                       double *
                                             edegdltptr,
                       SCOTCH_Num *
                                             ndegminptr,
                       SCOTCH_Num *
                                             ndegmaxptr,
                       double *
                                             ndegavgptr,
                       double *
                                             ndegdltptr)
scotchfmeshstat (doubleprecision (*)
                                        meshdat,
                  integer*num
                                        vnlomin.
                  integer*num
                                        vnlomax,
                  integer*num
                                        vnlosum,
                  doubleprecision
                                        vnloavg,
                                        vnlodlt,
                  doubleprecision
                  integer*num
                                         edegmin,
                  \verb"integer*" num
                                         edegmax,
                  doubleprecision
                                         edegavg,
                  doubleprecision
                                         edegdlt,
                  integer*num
                                        ndegmin,
                  integer*num
                                        ndegmax,
                  doubleprecision
                                        ndegavg,
                  doubleprecision
                                        ndegdlt)
```

## Description

The SCOTCH\_meshStat routine produces some statistics regarding the mesh structure pointed to by meshptr. vnlomin, vnlomax, vnlosum, vnloavg and vnlodlt are the minimum node vertex load, the maximum node vertex load, the sum of all node vertex loads, the average node vertex load, and the variance of the node vertex loads, respectively. edegmin, edegmax, edegavg and edegdlt are the minimum element vertex degree, the maximum element vertex degree, the average element vertex degree, and the variance of the element

vertex degrees, respectively. ndegmin, ndegmax, ndegavg and ndegdlt are the minimum element vertex degree, the maximum element vertex degree, the average element vertex degree, and the variance of the element vertex degrees, respectively.

# 8.12 High-level mesh ordering routines

This routine provides high-level functionality and frees the user from the burden of calling in sequence several of the low-level routines described afterward.

### 8.12.1 SCOTCH\_meshOrder

### **Synopsis**

```
int SCOTCH_meshOrder (const SCOTCH_Mesh *
                                             meshptr,
                      const SCOTCH_Strat *
                                             straptr,
                      SCOTCH_Num *
                                             permtab,
                      SCOTCH_Num *
                                             peritab,
                      SCOTCH_Num *
                                             cblkptr,
                      SCOTCH_Num *
                                             rangtab,
                      SCOTCH_Num *
                                              treetab)
scotchfmeshorder (doubleprecision (*)
                                         meshdat,
                  doubleprecision (*)
                                         stradat,
                  integer*num (*)
                                         permtab,
                  integer*num (*)
                                         peritab,
                  integer*num
                                         cblknbr,
                  integer*num (*)
                                         rangtab,
                  integer*num (*)
                                         treetab,
                  integer
                                         ierr)
```

## Description

The SCOTCH\_meshOrder routine computes a block ordering of the unknowns of the symmetric sparse matrix the adjacency structure of which is represented by the elements that connect the nodes of the source mesh structure pointed to by meshptr, using the ordering strategy pointed to by stratptr, and returns ordering data in the scalar pointed to by cblkptr and the four arrays permtab, peritab, rangtab and treetab.

The permtab, peritab, rangtab and treetab arrays should have been previously allocated, of a size sufficient to hold as many SCOTCH\_Num integers as there are node vertices in the source mesh, plus one in the case of rangtab. Any of the five output fields can be set to NULL if the corresponding information is not needed. Since, in Fortran, there is no null reference, passing a reference to meshptr in these fields will have the same effect.

On return, permtab holds the direct permutation of the unknowns, that is, node vertex i of the original mesh has index permtab[i] in the reordered mesh, while peritab holds the inverse permutation, that is, node vertex i in the reordered mesh had index peritab[i] in the original mesh. All of these indices are numbered according to the base value of the source mesh:

permutation indices are numbered from  $\min(\text{velmbas}, \text{vnodbas})$  to  $\text{vnodnbr} + \min(\text{velmbas}, \text{vnodbas}) - 1$ , that is, from 0 to vnodnbr - 1 if the mesh base is 0, and from 1 to vnodnbr if the mesh base is 1. The base value for mesh orderings is taken as  $\min(\text{velmbas}, \text{vnodbas})$ , and not just as vnodbas, such that orderings that are computed on some mesh have exactly the same index range as orderings that would be computed on the graph obtained from the original mesh by means of the SCOTCH\_meshGraph routine.

The three other result fields, \*cblkptr, rangtab and treetab, contain data related to the block structure. \*cblkptr holds the number of column blocks of the produced ordering, and rangtab holds the starting indices of each of the permuted column blocks, in increasing order, so that column block i starts at index rangtab [i] and ends at index (rangtab[i+1]-1), inclusive, in the new ordering. treetab holds the separators tree structure, that is, treetab [i] is the index of the father of column block i in the separators tree, or -1 if column block i is the root of the separators tree. Please refer to Section 8.2.5 for more information.

### Return values

SCOTCH\_meshOrder returns 0 if the ordering of the mesh has been successfully computed, and 1 else. In this last case, the rangtab, permtab, and peritab arrays may however have been partially or completely filled, but their contents are not significant.

# 8.13 Low-level mesh ordering routines

All of the following routines operate on a SCOTCH\_Ordering structure that contains references to the permutation arrays to be filled during the mesh ordering process.

# 8.13.1 SCOTCH\_meshOrderCheck

# Synopsis

# Description

The SCOTCH\_meshOrderCheck routine checks the consistency of the given SCOTCH\_Ordering structure pointed to by ordeptr.

### Return values

SCOTCH\_meshOrderCheck returns 0 if ordering data are consistent, and 1 else.

### 8.13.2 SCOTCH\_meshOrderCompute

The SCOTCH\_meshOrderCompute routine computes a block ordering of the mesh structure pointed to by grafptr, using the mapping strategy pointed to by stratptr, and stores its result in the ordering structure pointed to by ordeptr.

On return, the ordering structure holds a block ordering of the given mesh (see section 8.13.4 for a description of the ordering fields).

#### Return values

SCOTCH\_meshOrderCompute returns 0 if the ordering has been successfully computed, and 1 else. In this latter case, the ordering arrays may however have been partially or completely filled, but their contents are not significant.

### 8.13.3 SCOTCH\_meshOrderExit

## Synopsis

# Description

The SCOTCH\_meshOrderExit function frees the contents of a SCOTCH\_Ordering structure previously initialized by SCOTCH\_meshOrderInit. All subsequent calls to SCOTCH\_meshOrder\* routines other than SCOTCH\_meshOrderInit, using this structure as parameter, may yield unpredictable results.

## 8.13.4 SCOTCH\_meshOrderInit

```
scotchfmeshorderinit (doubleprecision (*)
                                            meshdat,
                      doubleprecision (*)
                                            ordedat,
                      integer*num (*)
                                            permtab,
                      integer*num (*)
                                            peritab,
                      integer*num
                                            cblknbr,
                      integer*num (*)
                                            rangtab,
                      integer*num (*)
                                            treetab,
                      integer
                                            ierr)
```

The SCOTCH\_meshOrderInit routine fills the ordering structure pointed to by ordeptr with all of the data that are passed to it. Thus, all subsequent calls to ordering routines such as SCOTCH\_meshOrderCompute, using this ordering structure as parameter, will place ordering results in fields permtab, peritab, \*cblkptr, rangtab or treetab, if they are not set to NULL.

permtab is the ordering permutation array, of size vnodnbr, peritab is the inverse ordering permutation array, of size vnodnbr, cblkptr is the pointer to a SCOTCH\_Num that will receive the number of produced column blocks, rangtab is the array that holds the column block span information, of size vnodnbr+1, and treetab is the array holding the structure of the separators tree, of size vnodnbr. See the above manual page of SCOTCH\_meshOrder, as well as section 8.2.5, for an explanation of the semantics of all of these fields.

The SCOTCH\_meshOrderInit routine should be the first function to be called upon a SCOTCH\_Ordering structure for ordering meshes. When the ordering structure is no longer of use, the SCOTCH\_meshOrderExit function must be called, in order to to free its internal structures.

# Return values

SCOTCH\_meshOrderInit returns 0 if the ordering structure has been successfully initialized, and 1 else.

## 8.13.5 SCOTCH\_meshOrderSave

### **Synopsis**

## Description

The SCOTCH\_meshOrderSave routine saves the contents of the SCOTCH\_Ordering structure pointed to by ordeptr to stream stream, in the SCOTCH ordering format (see section 6.6).

### Return values

SCOTCH\_meshOrderSave returns 0 if the ordering structure has been successfully written to stream, and 1 else.

### 8.13.6 SCOTCH\_meshOrderSaveMap

### **Synopsis**

# Description

The SCOTCH\_meshOrderSaveMap routine saves the block partitioning data associated with the SCOTCH\_Ordering structure pointed to by ordeptr to stream stream, in the SCOTCH mapping format (see section 6.5). A target domain number is associated with every block, such that all node vertices belonging to the same block are shown as belonging to the same target vertex.

This mapping file can then be used by the gout program (see section 7.3.12) to produce pictures showing the different separators and blocks. Since gout only takes graphs as input, the mesh has to be converted into a graph by means of the gmk\_msh program (see section 7.3.8).

### Return values

SCOTCH\_meshOrderSaveMap returns 0 if the ordering structure has been successfully written to stream, and 1 else.

## 8.13.7 SCOTCH\_meshOrderSaveTree

## Synopsis

### Description

The SCOTCH\_meshOrderSaveTree routine saves the tree hierarchy information associated with the SCOTCH\_Ordering structure pointed to by ordeptr to stream stream.

The format of the tree output file resembles the one of a mapping or ordering file: it is made up of as many lines as there are node vertices in the ordering. Each of these lines holds two integer numbers. The first one is the index or the label of the node vertex, starting from baseval, and the second one is the index of its parent node in the separators tree, or -1 if the vertex belongs to a root node.

Fortran users must use the PXFFILENO or FNUM functions to obtain the number of the Unix file descriptor fildes associated with the logical unit of the tree mapping file.

### Return values

SCOTCH\_meshOrderSaveTree returns 0 if the separators tree structure has been successfully written to stream, and 1 else.

# 8.14 Strategy handling routines

### 8.14.1 SCOTCH\_stratAlloc

Synopsis

```
SCOTCH_Strat * SCOTCH_stratAlloc (void)
```

### Description

The SCOTCH\_stratAlloc function allocates a memory area of a size sufficient to store a SCOTCH\_Strat structure. It is the user's responsibility to free this memory when it is no longer needed, using the SCOTCH\_memFree routine. The allocated space must be initialized before use, by means of the SCOTCH\_strat Init routine.

### Return values

SCOTCH\_stratAlloc returns the pointer to the memory area if it has been successfully allocated, and NULL else.

### 8.14.2 SCOTCH\_stratExit

### Synopsis

```
void SCOTCH_stratExit (SCOTCH_Strat * archptr)
scotchfstratexit (doubleprecision (*) stradat)
```

### Description

The SCOTCH\_stratExit function frees the contents of a SCOTCH\_Strat structure previously initialized by SCOTCH\_stratInit. All subsequent calls to

SCOTCH\_strat routines other than SCOTCH\_stratInit, using this structure as parameter, may yield unpredictable results.

### 8.14.3 SCOTCH\_stratInit

### **Synopsis**

# Description

The SCOTCH\_stratInit function initializes a SCOTCH\_Strat structure so as to make it suitable for future operations. It should be the first function to be called upon a SCOTCH\_Strat structure. When the strategy data is no longer of use, call function SCOTCH\_stratExit to free its internal structures.

#### Return values

SCOTCH\_stratInit returns 0 if the strategy structure has been successfully initialized, and 1 else.

### 8.14.4 SCOTCH\_stratSave

### Synopsis

## Description

The SCOTCH\_stratSave routine saves the contents of the SCOTCH\_Strat structure pointed to by straptr to stream stream, in the form of a text string. The methods and parameters of the strategy string depend on the type of the strategy, that is, whether it is a bipartitioning, mapping, or ordering strategy, and to which structure it applies, that is, graphs or meshes.

Fortran users must use the PXFFILENO or FNUM functions to obtain the number of the Unix file descriptor fildes associated with the logical unit of the output file.

# Return values

SCOTCH\_stratSave returns 0 if the strategy string has been successfully written to stream, and 1 else.

# 8.15 Strategy creation routines

Strategy creation routines parse the user-provided strategy string and populate the given opaque strategy object with a tree-shaped structure that represents the parsed expression. It is this structure that will be later traversed by the generic routines for partitioning, mapping or ordering, so as to determine which specific partitioning, mapping or ordering method to be called on a subgraph being considered.

Because strategy creation routines call third-party lexical analyzers that may have been implemented in a non-reentrant way, no guarantee is given on the reentrance of these routines. Consequently, strategy creation routines that might be called simultaneously by multiple threads should be protected by a mutex.

### 8.15.1 SCOTCH\_stratGraphBipart

### **Synopsis**

### Description

The SCOTCH\_stratGraphBipart routine fills the strategy structure pointed to by straptr with the graph bipartitioning strategy string pointed to by string. From this point, the strategy structure can only be used as a graph bipartitioning strategy, to be used by function SCOTCH\_archBuild, for instance.

When using the C interface, the array of characters pointed to by string must be null-terminated.

### Return values

SCOTCH\_stratGraphBipart returns 0 if the strategy string has been successfully set, and 1 else.

### 8.15.2 SCOTCH\_stratGraphClusterBuild

The SCOTCH\_stratGraphClusterBuild routine fills the strategy structure pointed to by straptr with a default clustering strategy tuned according to the preference flags passed as flagval, the maximum cluster vertex weight pwgtmax, the minimum edge density densmin, and the bipartition imbalance ratio bbalval. From this point, the strategy structure can only be used as a mapping strategy, to be used by a mapping function such as SCOTCH\_graph Map.

Recursive bipartitioning will be applied to the graph, every bipartition allowing for an imbalance tolerance of bbalval. Recursion will stop if either cluster size becomes smaller than pwgtmax, or cluster edge density becomes higher than densmin, which represents the fraction of edges internal to the cluster with respect to a complete graph. See Section 8.3.1 for a description of the available flags.

## Return values

 ${\tt SCOTCH\_stratGraphClusterBuild}$  returns 0 if the strategy string has been successfully set, and 1 else.

# 8.15.3 SCOTCH\_stratGraphMap

### Synopsis

# Description

The SCOTCH\_stratGraphMap routine fills the strategy structure pointed to by straptr with the graph mapping strategy string pointed to by string. From this point, the strategy structure can only be used as a mapping strategy, to be used by function SCOTCH\_graphMap, for instance.

When using the C interface, the array of characters pointed to by string must be null-terminated.

### Return values

SCOTCH\_stratGraphMap returns 0 if the strategy string has been successfully set, and 1 else.

# 8.15.4 SCOTCH\_stratGraphMapBuild

### **Synopsis**

```
int SCOTCH_stratGraphMapBuild (SCOTCH_Strat *
                                                 straptr,
                               const SCOTCH_Num flagval,
                               const SCOTCH_Num
                                                 partnbr,
                               const double
                                                 balrat)
scotchfstratgraphmapbuild (doubleprecision (*)
                                                 stradat,
                           integer*num
                                                 flagval,
                           integer*num
                                                 partnbr,
                           doubleprecision
                                                 balrat,
                           integer
                                                 ierr)
```

## Description

The SCOTCH\_stratGraphMapBuild routine fills the strategy structure pointed to by straptr with a default mapping strategy tuned according to the preference flags passed as flagval and to the desired number of parts partnbr and imbalance ratio balrat. From this point, the strategy structure can only be used as a mapping strategy, to be used by function SCOTCH\_graph Map, for instance. See Section 8.3.1 for a description of the available flags.

### Return values

SCOTCH\_stratGraphMapBuild returns 0 if the strategy string has been successfully set, and 1 else.

## 8.15.5 SCOTCH\_stratGraphPartOvl

### Synopsis

# Description

The SCOTCH\_stratGraphPartOvl routine fills the strategy structure pointed to by straptr with the graph partitioning with overlap strategy string pointed to by string. From this point, the strategy structure can only be used as a partitioning with overlap strategy, to be used by function SCOTCH\_graphPart Ovl only.

When using the C interface, the array of characters pointed to by string must be null-terminated.

### Return values

SCOTCH\_stratGraphPartOvl returns 0 if the strategy string has been successfully set, and 1 else.

## 8.15.6 SCOTCH\_stratGraphPartOvlBuild

## **Synopsis**

```
int SCOTCH_stratGraphPartOvlBuild (SCOTCH_Strat *
                                                     straptr,
                                   const SCOTCH_Num flagval,
                                   const SCOTCH_Num
                                                     partnbr,
                                   const double
                                                     balrat)
scotchfstratgraphpartovlbuild (doubleprecision (*)
                                                    stradat,
                               integer*num
                                                    flagval,
                               integer*num
                                                    partnbr,
                               doubleprecision
                                                    balrat,
                               integer
                                                     ierr)
```

# Description

The SCOTCH\_stratGraphPartOvlBuild routine fills the strategy structure pointed to by straptr with a default partitioning with overlap strategy tuned according to the preference flags passed as flagval and to the desired number of parts partnbr and imbalance ratio balrat. From this point, the strategy structure can only be used as a partitioning with overlap strategy, to be used by function SCOTCH\_graphPartOvl only. See Section 8.3.1 for a description of the available flags.

# Return values

SCOTCH\_stratGraphPartOvlBuild returns 0 if the strategy string has been successfully set, and 1 else.

# 8.15.7 SCOTCH\_stratGraphOrder

# Synopsis

# Description

The SCOTCH\_stratGraphOrder routine fills the strategy structure pointed to by straptr with the graph ordering strategy string pointed to by string. From this point, the strategy structure can only be used as a graph ordering strategy, to be used by function SCOTCH\_graphOrder, for instance.

When using the C interface, the array of characters pointed to by string must be null-terminated.

### Return values

SCOTCH\_stratGraphOrder returns 0 if the strategy string has been successfully set, and 1 else.

# 8.15.8 SCOTCH\_stratGraphOrderBuild

## **Synopsis**

### Description

The SCOTCH\_stratGraphOrderBuild routine fills the strategy structure pointed to by straptr with a default sequential ordering strategy tuned according to the preference flags passed as flagval and to the desired nested dissection imbalance ratio balrat. From this point, the strategy structure can only be used as an ordering strategy, to be used by function SCOTCH\_graph Order, for instance.

See Section 8.3.1 for a description of the available flags. When any of the SCOTCH\_STRATLEVELMIN or SCOTCH\_STRATLEVELMAX flags is set, the levlnbr parameter is taken into account.

# Return values

SCOTCH\_stratGraphOrderBuild returns 0 if the strategy string has been successfully set, and 1 else.

## 8.15.9 SCOTCH\_stratMeshOrder

# Synopsis

# Description

The SCOTCH\_stratMeshOrder routine fills the strategy structure pointed to by straptr with the mesh ordering strategy string pointed to by string. From this point, strategy strat can only be used as a mesh ordering strategy, to be used by function SCOTCH\_meshOrder, for instance.

When using the C interface, the array of characters pointed to by string must be null-terminated.

### Return values

SCOTCH\_stratMeshOrder returns 0 if the strategy string has been successfully set, and 1 else.

### 8.15.10 SCOTCH\_stratMeshOrderBuild

## Synopsis

### Description

The SCOTCH\_stratMeshOrderBuild routine fills the strategy structure pointed to by straptr with a default ordering strategy tuned according to the preference flags passed as flagval and to the desired nested dissection imbalance ratio balrat. From this point, the strategy structure can only be used as an ordering strategy, to be used by function SCOTCH\_meshOrder, for instance. See Section 8.3.1 for a description of the available flags.

## Return values

 ${\tt SCOTCH\_stratMesdOrderBuild}$  returns 0 if the strategy string has been successfully set, and 1 else.

# 8.16 Geometry handling routines

Since the Scotch project is based on algorithms that rely on topology data only, geometry data do not play an important role in the LIBSCOTCH library. They are only relevant to programs that display graphs, such as the gout program. However, since all routines that are used by the programs of the Scotch distributions have an interface in the LIBSCOTCH library, there exist geometry handling routines in it, which manipulate SCOTCH\_Geom structures.

Apart from the routines that create, destroy or access SCOTCH\_Geom structures, all of the routines in this section are input/output routines, which read or write both SCOTCH\_Graph and SCOTCH\_Geom structures. We have chosen to define the interface of the geometry-handling routines such that they also handle graph or mesh topology because some external file formats mix these data, and that we wanted our routines to be able to read their data on the fly from streams that can

only be read once, such as communication pipes. Having both aspects taken into account in a single call makes the writing of file conversion tools, such as gcv and mcv, very easy. When the file format from which to read or into which to write mixes both sorts of data, the geometry file pointer can be set to NULL, as it will not be used.

### 8.16.1 SCOTCH\_geomAlloc

# Synopsis

```
SCOTCH_Geom * SCOTCH_geomAlloc (void)
```

## Description

The SCOTCH\_geomAlloc function allocates a memory area of a size sufficient to store a SCOTCH\_Geom structure. It is the user's responsibility to free this memory when it is no longer needed, using the SCOTCH\_memFree routine. The allocated space must be initialized before use, by means of the SCOTCH\_geom Init routine.

#### Return values

SCOTCH\_geomAlloc returns the pointer to the memory area if it has been successfully allocated, and NULL else.

# 8.16.2 SCOTCH\_geomInit

## Synopsis

# Description

The SCOTCH\_geomInit function initializes a SCOTCH\_Geom structure so as to make it suitable for future operations. It should be the first function to be called upon a SCOTCH\_Geom structure. When the geometrical data is no longer of use, call function SCOTCH\_geomExit to free its internal structures.

# Return values

SCOTCH\_geomInit returns 0 if the geometrical structure has been successfully initialized, and 1 else.

# 8.16.3 SCOTCH\_geomExit

```
void SCOTCH_geomExit (SCOTCH_Geom * geomptr)
scotchfgeomexit (doubleprecision (*) geomdat)
```

The SCOTCH\_geomExit function frees the contents of a SCOTCH\_Geom structure previously initialized by SCOTCH\_geomInit. All subsequent calls to SCOTCH\_\*Geom\* routines other than SCOTCH\_geomInit, using this structure as parameter, may yield unpredictable results.

### 8.16.4 SCOTCH\_geomData

# Synopsis

# Description

The SCOTCH\_geomData routine is a multiple accessor to the contents of SCOTCH\_Geom structures.

dimptr is the pointer to a location that will hold the number of dimensions of the graph vertex or mesh node vertex coordinates, and will therefore be equal to 1, 2 or 3. geomtab is the pointer to a location that will hold the reference to the geometry coordinates, as defined in section 8.2.4.

Any of these pointers can be set to NULL on input if the corresponding information is not needed. Else, the reference to a dummy area can be provided, where all unwanted data will be written.

Since there are no pointers in Fortran, a specific mechanism is used to allow users to access the coordinate array. The scotchfgeomdata routine is passed an integer array, the first element of which is used as a base address from which all other array indices are computed. Therefore, instead of returning a reference, the routine returns an integer, which represents the starting index of the coordinate array with respect to the base input array. For instance, if some base array myarray(1) is passed as parameter indxtab, then the first cell of array geomtab will be accessible as myarray(geomidx). In order for this feature to behave properly, the indxtab array must be double-precisionaligned with the geometry array. This is automatically enforced on most systems, but some care should be taken on systems that allow one to access data that is not double-aligned. On such systems, declaring the array after a dummy doubleprecision array can coerce the compiler into enforcing the proper alignment. Also, on 32\_64 architectures, such indices can be larger than the size of a regular INTEGER. This is why the indices to be returned

are defined by means of a specific integer type. See Section 8.1.5 for more information on this issue.

## 8.16.5 SCOTCH\_graphGeomLoadChac

### **Synopsis**

```
int SCOTCH_graphGeomLoadChac (SCOTCH_Graph *
                                              grafptr,
                              SCOTCH_Geom *
                                              geomptr,
                              FILE *
                                              grafstream,
                              FILE *
                                              geomstream,
                              const char *
                                              string)
scotchfgraphgeomloadchac (doubleprecision (*) grafdat,
                          doubleprecision (*) geomdat,
                                                graffildes,
                          integer
                                                geomfildes,
                          integer
                          character (*)
                                                string)
```

### Description

The SCOTCH\_graphGeomLoadChac routine fills the SCOTCH\_Graph structure pointed to by grafptr with the source graph description available from stream grafstream in the Chaco graph format [25]. Since this graph format does not handle geometry data, the geomptr and geomstream fields are not used, as well as the string field.

Fortran users must use the PXFFILENO or FNUM functions to obtain the number of the Unix file descriptor graffildes associated with the logical unit of the graph file.

## Return values

SCOTCH\_graphGeomLoadChac returns 0 if the graph structure has been successfully allocated and filled with the data read, and 1 else.

# 8.16.6 SCOTCH\_graphGeomSaveChac

```
int SCOTCH_graphGeomSaveChac (const SCOTCH_Graph *
                                                     grafptr,
                              const SCOTCH_Geom *
                                                     geomptr,
                              FILE *
                                                     grafstream,
                              FILE *
                                                     geomstream,
                              const char *
                                                     string)
scotchfgraphgeomsavechac (doubleprecision (*)
                                                grafdat,
                          doubleprecision (*)
                                                geomdat,
                          integer
                                                graffildes,
                          integer
                                                geomfildes,
                          character (*)
                                                string)
```

The SCOTCH\_graphGeomSaveChac routine saves the contents of the SCOTCH\_Graph structure pointed to by grafptr to stream grafstream, in the CHACO graph format [25]. Since this graph format does not handle geometry data, the geomptr and geomstream fields are not used, as well as the string field.

Fortran users must use the PXFFILENO or FNUM functions to obtain the number of the Unix file descriptor graffildes associated with the logical unit of the graph file.

### Return values

SCOTCH\_graphGeomSaveChac returns 0 if the graph structure has been successfully written to grafstream, and 1 else.

# $8.16.7 \quad {\tt SCOTCH\_graphGeomLoadHabo}$

# **Synopsis**

```
int SCOTCH_graphGeomLoadHabo (SCOTCH_Graph *
                                               grafptr,
                              SCOTCH_Geom *
                                               geomptr,
                              FILE *
                                               grafstream,
                              FILE *
                                               geomstream,
                               const char *
                                               string)
scotchfgraphgeomloadhabo (doubleprecision (*)
                                                 grafdat,
                           doubleprecision (*)
                                                geomdat,
                                                 graffildes,
                           integer
                           integer
                                                 geomfildes,
                           character (*)
                                                 string)
```

## Description

The SCOTCH\_graphGeomLoadHabo routine fills the SCOTCH\_Graph structure pointed to by grafptr with the source graph description available from stream grafstream in the Harwell-Boeing square assembled matrix format [10]. Since this graph format does not handle geometry data, the geomptr and geom stream fields are not used. Since multiple graph structures can be encoded sequentially within the same file, the string field contains the string representation of an integer number that codes the rank of the graph to read within the Harwell-Boeing file. It is equal to "0" in most cases.

Fortran users must use the PXFFILENO or FNUM functions to obtain the number of the Unix file descriptor graffildes associated with the logical unit of the graph file.

## Return values

SCOTCH\_graphGeomLoadHabo returns 0 if the graph structure has been successfully allocated and filled with the data read, and 1 else.

## 8.16.8 SCOTCH\_graphGeomLoadScot

### **Synopsis**

```
int SCOTCH_graphGeomLoadScot (SCOTCH_Graph *
                                               grafptr,
                              SCOTCH_Geom *
                                               geomptr,
                              FILE *
                                               grafstream,
                              FILE *
                                               geomstream,
                              const char *
                                               string)
scotchfgraphgeomloadscot (doubleprecision (*)
                                                grafdat,
                          doubleprecision (*)
                                                geomdat,
                          integer
                                                 graffildes,
                          integer
                                                geomfildes,
                          character (*)
                                                string)
```

# Description

The SCOTCH\_graphGeomLoadScot routine fills the SCOTCH\_Graph and SCOTCH\_Geom structures pointed to by grafptr and geomptr with the source graph description and geometry data available from streams grafstream and geom stream in the SCOTCH graph and geometry formats (see sections 6.1 and 6.3, respectively). The string field is not used.

Fortran users must use the PXFFILENO or FNUM functions to obtain the numbers of the Unix file descriptors graffildes and geomfildes associated with the logical units of the graph and geometry files.

## Return values

SCOTCH\_graphGeomLoadScot returns 0 if the graph topology and geometry have been successfully allocated and filled with the data read, and 1 else.

## 8.16.9 SCOTCH\_graphGeomSaveScot

# Synopsis

```
int SCOTCH_graphGeomSaveScot (const SCOTCH_Graph *
                                                     grafptr,
                              const SCOTCH_Geom *
                                                     geomptr,
                              FILE *
                                                     grafstream,
                              FILE *
                                                     geomstream,
                              const char *
                                                     string)
scotchfgraphgeomsavescot (doubleprecision (*) grafdat,
                          doubleprecision (*)
                                                geomdat,
                          integer
                                                graffildes,
                                                geomfildes,
                          integer
                          character (*)
                                                string)
```

# Description

The SCOTCH\_graphGeomSaveScot routine saves the contents of the SCOTCH\_Graph and SCOTCH\_Geom structures pointed to by grafptr and geomptr to streams grafstream and geomstream, in the SCOTCH graph and geometry formats (see sections 6.1 and 6.3, respectively). The string field is not used.

Fortran users must use the PXFFILENO or FNUM functions to obtain the numbers of the Unix file descriptors graffildes and geomfildes associated with the logical units of the graph and geometry files.

### Return values

SCOTCH\_graphGeomSaveScot returns 0 if the graph topology and geometry have been successfully written to grafstream and geomstream, and 1 else.

#### 8.16.10 SCOTCH\_meshGeomLoadHabo

### **Synopsis**

```
int SCOTCH_meshGeomLoadHabo (SCOTCH_Mesh * meshptr,
                            SCOTCH_Geom * geomptr,
                            FILE *
                                           meshstream,
                            FILE *
                                           geomstream,
                            const char *
                                           string)
scotchfmeshgeomloadhabo (doubleprecision (*)
                                              meshdat,
                         doubleprecision (*) geomdat,
                         integer
                                              meshfildes,
                         integer
                                              geomfildes,
                         character (*)
                                              string)
```

## Description

The SCOTCH\_meshGeomLoadHabo routine fills the SCOTCH\_Mesh structure pointed to by meshptr with the source mesh description available from stream meshstream in the Harwell-Boeing square elemental matrix format [10]. Since this mesh format does not handle geometry data, the geomptr and geom stream fields are not used. Since multiple mesh structures can be encoded sequentially within the same file, the string field contains the string representation of an integer number that codes the rank of the mesh to read within the Harwell-Boeing file. It is equal to "0" in most cases.

Fortran users must use the PXFFILENO or FNUM functions to obtain the number of the Unix file descriptor meshfildes associated with the logical unit of the mesh file.

### Return values

SCOTCH\_meshGeomLoadHabo returns 0 if the mesh structure has been successfully allocated and filled with the data read, and 1 else.

### 8.16.11 SCOTCH\_meshGeomLoadScot

```
int SCOTCH_meshGeomLoadScot (SCOTCH_Mesh *
                                            meshptr,
                             SCOTCH_Geom *
                                           geomptr,
                             FILE *
                                            meshstream,
                             FILE *
                                            geomstream,
                             const char * string)
scotchfmeshgeomloadscot (doubleprecision (*)
                                              meshdat,
                         doubleprecision (*)
                                              geomdat,
                         integer
                                              meshfildes,
                         integer
                                               geomfildes,
                         character (*)
                                               string)
```

The SCOTCH\_meshGeomLoadScot routine fills the SCOTCH\_Mesh and SCOTCH\_Geom structures pointed to by meshptr and geomptr with the source mesh description and node geometry data available from streams meshstream and geomstream in the SCOTCH mesh and geometry formats (see sections 6.2 and 6.3, respectively). The string field is not used.

Fortran users must use the PXFFILENO or FNUM functions to obtain the numbers of the Unix file descriptors meshfildes and geomfildes associated with the logical units of the mesh and geometry files.

#### Return values

SCOTCH\_meshGeomLoadScot returns 0 if the mesh topology and node geometry have been successfully allocated and filled with the data read, and 1 else.

# 8.16.12 SCOTCH\_meshGeomSaveScot

# Synopsis

```
int SCOTCH_meshGeomSaveScot (const SCOTCH_Mesh * meshptr,
                             const SCOTCH_Geom *
                                                  geomptr,
                             FILE *
                                                  meshstream,
                            FILE *
                                                  geomstream,
                             const char *
                                                  string)
scotchfmeshgeomsavescot (doubleprecision (*)
                                              meshdat,
                         doubleprecision (*)
                                              geomdat,
                         integer
                                              meshfildes,
                         integer
                                              geomfildes,
                         character (*)
                                              string)
```

### Description

The SCOTCH\_meshGeomSaveScot routine saves the contents of the SCOTCH\_Mesh and SCOTCH\_Geom structures pointed to by meshptr and geomptr to streams meshstream and geomstream, in the SCOTCH mesh and geometry formats (see sections 6.2 and 6.3, respectively). The string field is not used.

Fortran users must use the PXFFILENO or FNUM functions to obtain the numbers of the Unix file descriptors meshfildes and geomfildes associated with the logical units of the mesh and geometry files.

### Return values

SCOTCH\_meshGeomSaveScot returns 0 if the mesh topology and node geometry have been successfully written to meshstream and geomstream, and 1 else.

# 8.17 Other data structure handling routines

## 8.17.1 SCOTCH\_mapAlloc

Synopsis

SCOTCH\_Mapping \* SCOTCH\_mapAlloc (void)

### Description

The SCOTCH\_mapAlloc function allocates a memory area of a size sufficient to store a SCOTCH\_Mapping structure. It is the user's responsibility to free this memory when it is no longer needed, using the SCOTCH\_memFree routine.

#### Return values

SCOTCH\_mapAlloc returns the pointer to the memory area if it has been successfully allocated, and NULL else.

## 8.17.2 SCOTCH\_orderAlloc

Synopsis

SCOTCH\_Ordering \* SCOTCH\_orderAlloc (void)

### Description

The SCOTCH\_orderAlloc function allocates a memory area of a size sufficient to store a SCOTCH\_Ordering structure. It is the user's responsibility to free this memory when it is no longer needed, using the SCOTCH\_memFree routine.

## Return values

SCOTCH\_orderAlloc returns the pointer to the memory area if it has been successfully allocated, and NULL else.

# 8.18 Error handling routines

The handling of errors that occur within library routines is often difficult, because library routines should be able to issue error messages that help the application programmer to find the error, while being compatible with the way the application handles its own errors.

To match these two requirements, all the error and warning messages produced by the routines of the LIBSCOTCH library are issued using the user-definable variable-length argument routines SCOTCH\_errorPrint and SCOTCH\_errorPrintW. Thus, one can redirect these error messages to his own error handling routines, and can choose if he wants his program to terminate on error or to resume execution after the erroneous function has returned.

In order to free the user from the burden of writing a basic error handler from scratch, the libscotcherr.a library provides error routines that print error messages on the standard error stream stderr and return control to the application. Application programmers who want to take advantage of them have to add-lscotcherr to the list of arguments of the linker, after the -lscotch argument.

### 8.18.1 SCOTCH\_errorPrint

## Synopsis

```
void SCOTCH_errorPrint (const char * const errstr, ...)
```

## Description

The SCOTCH\_errorPrint function is designed to output a variable-length argument error string to some stream.

### 8.18.2 SCOTCH\_errorPrintW

# **Synopsis**

```
void SCOTCH_errorPrintW (const char * const errstr, ...)
```

## Description

The SCOTCH\_errorPrintW function is designed to output a variable-length argument warning string to some stream.

# 8.18.3 SCOTCH\_errorProg

## Synopsis

```
void SCOTCH_errorProg (const char * progstr)
```

# Description

The SCOTCH\_errorProg function is designed to be called at the beginning of a program or of a portion of code to identify the place where subsequent errors take place. This routine is not reentrant, as it is only a minor help function. It is defined in libscotcherr.a and is used by the standalone programs of the SCOTCH distribution.

### 8.19 Miscellaneous routines

#### 8.19.1 SCOTCH\_memCur

Synopsis

```
SCOTCH_Idx SCOTCH_memCur (void)  scotchfmemcur (integer*idx memcur)
```

### Description

When SCOTCH is compiled with the COMMON\_MEMORY\_TRACE flag set, the SCOTCH\_memCur routine returns the amount of memory, in bytes, that is currently allocated by SCOTCH on the current processing element, either by itself or on the behalf of the user. Else, the routine returns -1.

The returned figure does not account for the memory that has been allocated by the user and made visible to Scotch by means of routines such as SCOTCH\_dgraphBuild calls. This memory is not under the control of Scotch, and it is the user's responsibility to free it after calling the relevant SCOTCH\_\* Exit routines.

Some third-party software used by SCOTCH, such as the strategy string parser, may allocate some memory for internal use and never free it. Consequently, there may be small discrepancies between memory occupation figures returned by SCOTCH and those returned by third-party tools. However, these discrepancies should not exceed a few kilobytes.

While memory occupation is internally recorded in a variable of type intptrt, it is output as a SCOTCH\_Idx for the sake of interface homogeneity, especially for Fortran. It is therefore the installer's responsibility to make sure that the support integer type of SCOTCH\_Idx is large enough to not overflow. See section 8.1.5 for more information.

#### 8.19.2 SCOTCH\_memFree

#### Synopsis

```
void SCOTCH_memFree (void * dataptr)
```

#### Description

The SCOTCH\_memFree routine frees the memory space allocated by routines such as SCOTCH\_graphAlloc, SCOTCH\_meshAlloc, or SCOTCH\_stratAlloc.

The standard free routine of the Libc must not be used for this purpose. Else, the allocated memory will not be considered as properly released by memory accounting routines SCOTCH\_memCur and SCOTCH\_memMax, and segmentation errors would happen when the COMMON\_MEMORY\_CHECK compile flag is set.

#### 8.19.3 SCOTCH\_memMax

### Synopsis

```
SCOTCH_Idx SCOTCH_memMax (void) scotchfmemmax (integer*idx memcur)
```

### Description

When SCOTCH is compiled with the COMMON\_MEMORY\_TRACE flag set, the SCOTCH\_memMax routine returns the maximum amount of memory, in bytes, ever allocated by SCOTCH on the current processing element, either by itself or on the behalf of the user. Else, the routine returns -1.

The returned figure does not account for the memory that has been allocated by the user and made visible to Scotch by means of routines such as SCOTCH\_dgraphBuild calls. This memory is not under the control of Scotch, and it is the user's responsibility to free it after calling the relevant SCOTCH\_\* Exit routines.

Some third-party software used by SCOTCH, such as the strategy string parser, may allocate some memory for internal use and never free it. Consequently, there may be small discrepancies between memory occupation figures returned by SCOTCH and those returned by third-party tools. However, these discrepancies should not exceed a few kilobytes.

While memory occupation is internally recorded in a variable of type intptrt, it is output as a SCOTCH\_Idx for the sake of interface homogeneity, especially for Fortran. It is therefore the installer's responsibility to make sure that the support integer type of SCOTCH\_Idx is large enough to not overflow. See section 8.1.5 for more information.

#### 8.19.4 SCOTCH\_numSizeof

#### Synopsis

```
int SCOTCH_numSizeof (void)
scotchfnumsizeof (integer size )
```

#### Description

The SCOTCH\_numSizeof routine returns the size, in bytes, of a SCOTCH\_Num. This information is useful to export the interface of the LIBSCOTCH to interpreted languages, without access to the "scotch.h" include file.

### 8.19.5 SCOTCH\_randomReset

### Synopsis

```
void SCOTCH_randomReset (void)
scotchfrandomreset ()
```

## Description

The SCOTCH\_randomReset routine resets the seed of the pseudo-random generator used by the graph partitioning routines of the LIBSCOTCH library. Two consecutive calls to the same LIBSCOTCH partitioning or ordering routines, separated by a call to SCOTCH\_randomReset, will always yield the same results.

### 8.19.6 SCOTCH\_randomSeed

### **Synopsis**

```
void SCOTCH_randomSeed (SCOTCH_Num seedval) scotchfrandomseed (integer*num seedval)
```

#### Description

The SCOTCH\_randomSeed routine sets to seedval the seed of the pseudorandom generator used internally by several algorithms of SCOTCH. All subsequent calls to SCOTCH\_randomReset will use this value to reset the pseudorandom generator.

This routine needs only to be used by users willing to evaluate the robustness and quality of partitioning algorithms with respect to the variability of random seeds. Else, depending whether SCOTCH has been compiled with any of the flags COMMON\_RANDOM\_FIXED\_SEED or SCOTCH\_DETERMINISTIC set or not, either the same pseudo-random seed will be always used, or a process-dependent seed will be used, respectively.

### 8.19.7 SCOTCH\_version

### Synopsis

### Description

The SCOTCH\_version routine writes the version, release and patchlevel numbers of the SCOTCH library that is currently being used, to integer values

\*versptr, \*relaptr and patcptr, respectively. This routine is mainly useful for applications willing to record runtime information, such as the library against which they are dynamically linked.

### 8.20 MeTiS compatibility library

The METIS compatibility library provides stubs which redirect some calls to METIS routines to the corresponding SCOTCH counterparts. In order to use this feature, the only thing to do is to re-link the existing software with the libscotchmetis library, and eventually with the original METIS library if the software uses METIS routines which do not need to have SCOTCH equivalents, such as graph transformation routines. In that latter case, the "-lscotchmetis" argument must be placed before the "-lmetis" one (and of course before the "-lscotch" one too), so that routines that are redefined by SCOTCH are chosen instead of their METIS counterpart. When no other METIS routines than the ones redefined by SCOTCH are used, the "-lmetis" argument can be omitted. See Section 10 for an example.

#### 8.20.1 METIS\_EdgeND

### **Synopsis**

```
void METIS_EdgeND (const SCOTCH_Num * const
                   const SCOTCH_Num * const xadj,
                   const SCOTCH_Num * const
                                             adjncy,
                   const SCOTCH_Num * const
                                             numflag,
                   const SCOTCH_Num * const options,
                   SCOTCH_Num * const
                                             perm,
                   SCOTCH_Num * const
                                             iperm)
metis_edgend (integer*num
              integer*num (*)
                               xadj,
              integer*num (*)
                                adjncy,
              integer*num
                                numflag,
              integer*num (*)
                                options,
              integer*num (*)
                                perm,
              integer*num (*)
                                iperm)
```

### Description

The METIS\_EdgeND function performs a nested dissection ordering of the graph passed as arrays xadj and adjncy, using the default SCOTCH ordering strategy. The options array is not used. The perm and iperm arrays have the opposite meaning as in SCOTCH: the METIS perm array holds what is called "inverse permutation" in SCOTCH, while iperm holds what is called "direct permutation" in SCOTCH.

While SCOTCH has also both node and edge separation capabilities, all of the three METIS stubs METIS\_EdgeND, METIS\_NodeND and METIS\_NodeWND call the same SCOTCH routine, which uses the SCOTCH default ordering strategy proved to be efficient in most cases.

#### 8.20.2 METIS\_NodeND

#### **Synopsis**

```
void METIS_NodeND (const SCOTCH_Num * const
                  const SCOTCH_Num * const xadj,
                   const SCOTCH_Num * const
                                            adjncy,
                   const SCOTCH_Num * const numflag,
                   const SCOTCH_Num * const options,
                   SCOTCH_Num * const
                                             perm,
                   SCOTCH_Num * const
                                             iperm)
metis_nodend (integer*num
                               n.
              integer*num (*)
                               xadj,
              integer*num (*)
                               adjncy,
              integer*num
                               numflag,
              integer*num (*)
                               options,
              integer*num (*)
                               perm,
              integer*num (*)
                               iperm)
```

#### Description

The METIS\_NodeND function performs a nested dissection ordering of the graph passed as arrays xadj and adjncy, using the default SCOTCH ordering strategy. The options array is not used. The perm and iperm arrays have the opposite meaning as in SCOTCH: the METIS perm array holds what is called "inverse permutation" in SCOTCH, while iperm holds what is called "direct permutation" in SCOTCH.

While SCOTCH has also both node and edge separation capabilities, all of the three METiS stubs METIS\_EdgeND, METIS\_NodeND and METIS\_NodeWND call the same SCOTCH routine, which uses the SCOTCH default ordering strategy proved to be efficient in most cases.

### 8.20.3 METIS\_NodeWND

### Synopsis

```
metis_nodwend (integer*num
                                 n,
               integer*num (*)
                                 xadj,
               integer*num (*)
                                 adjncy,
               integer*num (*)
                                 vwgt,
               integer*num
                                 numflag,
               integer*num (*)
                                 options,
               integer*num (*)
                                 perm,
               integer*num (*)
                                 iperm)
```

### Description

The METIS\_NodeWND function performs a nested dissection ordering of the graph passed as arrays xadj, adjncy and vwgt, using the default SCOTCH ordering strategy. The options array is not used. The perm and iperm arrays have the opposite meaning as in SCOTCH: the METIS perm array holds what is called "inverse permutation" in SCOTCH, while iperm holds what is called "direct permutation" in SCOTCH.

While SCOTCH has also both node and edge separation capabilities, all of the three METIS stubs METIS\_EdgeND, METIS\_NodeND and METIS\_NodeWND call the same SCOTCH routine, which uses the SCOTCH default ordering strategy proved to be efficient in most cases.

### 8.20.4 METIS\_PartGraphKway

### **Synopsis**

```
void METIS_PartGraphKway (const SCOTCH_Num * const
                          const SCOTCH_Num * const xadj,
                          const SCOTCH_Num * const adjncy,
                         const SCOTCH_Num * const
                                                    vwgt,
                          const SCOTCH_Num * const
                                                    adjwgt,
                          const SCOTCH_Num * const
                                                   wgtflag,
                          const SCOTCH_Num * const
                                                   numflag,
                         const SCOTCH_Num * const
                                                   nparts,
                          const SCOTCH_Num * const
                                                    options,
                         SCOTCH_Num * const
                                                    edgecut,
                         SCOTCH_Num * const
                                                    part)
metis_partgraphkway (integer*num
                                      n,
                    integer*num (*)
                                      xadj,
                     integer*num (*)
                                      adjncy,
                    integer*num (*)
                                      vwgt,
                     integer*num (*)
                                      adjwgt,
                    integer*num
                                      wgtflag,
                     integer*num
                                      numflag,
                    integer*num
                                      nparts,
                     integer*num (*)
                                      options,
                    integer*num
                                      edgecut,
                     integer*num (*)
                                      part)
```

#### Description

The METIS\_PartGraphKway function performs a mapping onto the complete graph of the graph represented by arrays xadj, adjncy, vwgt and adjwgt, using the default Scotch mapping strategy. The options array is not used. The part array has the same meaning as the parttab array of Scotch.

All of the three METIS stubs METIS\_PartGraphKway, METIS\_PartGraph Recursive and METIS\_PartGraphVKway call the same SCOTCH routine, which uses the SCOTCH default mapping strategy proved to be efficient in most cases.

### 8.20.5 METIS\_PartGraphRecursive

#### Synopsis

```
void METIS_PartGraphRecursive (const SCOTCH_Num * const n,
                              const SCOTCH_Num * const xadj,
                              const SCOTCH_Num * const adjncy,
                              const SCOTCH_Num * const vwgt,
                              const SCOTCH_Num * const adjwgt,
                              const SCOTCH_Num * const wgtflag,
                              const SCOTCH_Num * const numflag,
                              const SCOTCH_Num * const nparts,
                              const SCOTCH_Num * const options,
                              SCOTCH_Num * const
                                                       edgecut,
                              SCOTCH_Num * const
                                                       part)
metis_partgraphrecursive (integer*num
                         integer*num (*) xadj,
                         integer*num (*) adjncy,
                         integer*num (*)
                                          vwgt,
                         integer*num (*)
                                          adjwgt,
                         integer*num
                                          wgtflag,
                         integer*num
                                          numflag,
                         integer*num
                                          nparts,
                         integer*num (*)
                                          options,
                         integer*num
                                           edgecut,
                         integer*num (*) part)
```

### Description

The METIS\_PartGraphRecursive function performs a mapping onto the complete graph of the graph represented by arrays xadj, adjncy, vwgt and adjwgt, using the default Scotch mapping strategy. The options array is not used. The part array has the same meaning as the parttab array of Scotch. To date, the computation of the edgecut field requires extra processing, which increases running time to a small extent.

All of the three METIS stubs METIS\_PartGraphKway, METIS\_PartGraph Recursive and METIS\_PartGraphVKway call the same SCOTCH routine, which uses the SCOTCH default mapping strategy proved to be efficient in most cases.

#### 8.20.6 METIS\_PartGraphVKway

### **Synopsis**

```
void METIS_PartGraphVKway (const SCOTCH_Num * const
                           const SCOTCH_Num * const xadj,
                           const SCOTCH_Num * const
                                                    adjncy,
                           const SCOTCH_Num * const vwgt,
                           const SCOTCH_Num * const vsize,
                           const SCOTCH_Num * const wgtflag,
                           const SCOTCH_Num * const numflag,
                           const SCOTCH_Num * const nparts,
                           const SCOTCH_Num * const options,
                           SCOTCH_Num * const
                                                     volume,
                           SCOTCH_Num * const
                                                     part)
metis_partgraphvkway (integer*num
                      integer*num (*)
                                       xadj,
                      integer*num (*)
                                       adjncy,
                      integer*num (*)
                                        vwgt,
                      integer*num (*)
                                       vsize,
                      integer*num
                                       wgtflag,
                      integer*num
                                       numflag,
                      integer*num
                                       nparts,
                      integer*num (*)
                                       options,
                      integer*num
                                        volume,
                      integer*num (*)
                                       part)
```

### Description

The METIS\_PartGraphVKway function performs a mapping onto the complete graph of the graph represented by arrays xadj, adjncy, vwgt and vsize, using the default SCOTCH mapping strategy. The options array is not used. The part array has the same meaning as the parttab array of SCOTCH.

Since Scotch does not have methods for explicitely reducing the communication volume according to the metric of METIS\_PartGraphVKway, this routine creates a temporary edge weight array such that each edge (u,v) receives a weight equal to mboxvsize(u) + mboxvsize(v). Consequently, edges which are incident to highly communicating vertices will be less likely to be cut. However, the communication volume value returned by this routine is exactly the one which would be returned by METIS with respect to the output partition. Users interested in minimizing the exact communication volume should consider using hypergraphs, implemented in Scotch as meshes (see Section 8.2.3).

All of the three METIS\_PartGraphVKway, METIS\_PartGraphVKway and METIS\_PartGraphVKway call the same SCOTCH routine, which uses the SCOTCH default mapping strategy proved to be efficient in most cases.

### 9 Installation

Version 6.0 of the Scotch software package is distributed as free/libre software under the CeCILL-C free/libre software license [6], which is very similar to the GNU LGPL license. Therefore, it is no longer distributed as a set of binaries, but instead in the form of a source distribution, which can be downloaded from the Scotch web page at http://www.labri.fr/~pelegrin/scotch/.

All Scotch users are welcome to send an e-mail to the author so that they can be added to the Scotch mailing list, and be automatically informed of new releases and publications.

The extraction process will create a scotch\_6.0.4 directory, containing several subdirectories and files. Please refer to the files called LICENSE\_EN.txt or LICENCE\_FR.txt, as well as file INSTALL\_EN.txt, to see under which conditions your distribution of Scotch is licensed and how to install it.

#### 9.1 Thread issues

To enable the use of POSIX threads in some routines, the SCOTCH\_PTHREAD flag must be set. If your MPI implementation is not thread-safe, make sure this flag is not defined at compile time.

### 9.2 File compression issues

To enable on-the-fly compression and decompression of various formats, the relevant flags must be defined. These flags are COMMON\_FILE\_COMPRESS\_BZ2 for bzip2 (de)compression, COMMON\_FILE\_COMPRESS\_GZ for gzip (de)compression, and COMMON\_FILE\_COMPRESS\_LZMA for lzma decompression. Note that the corresponding development libraries must be installed on your system before compile time, and that compressed file handling can take place only on systems which support multi-threading or multi-processing. In the first case, you must set the SCOTCH\_PTHREAD flag in order to take advantage of these features.

On Linux systems, the development libraries to install are libbzip2\_1-devel for the bzip2 format, zlib1-devel for the gzip format, and liblzma0-devel for the lzma format. The names of the libraries may vary according to operating systems and library versions. Ask your system engineer in case of trouble.

### 9.3 Machine word size issues

The integer values handled by SCOTCH are based on the SCOTCH\_Num type, which equates by default to the int C type, corresponding to the INTEGER Fortran type, both of which being of machine word size. To coerce the length of the SCOTCH\_Num integer type to 32 or 64 bits, one can use the "-DINTSIZE32" or "-DINTSIZE64" flags, respectively, or else use the "-DINT=" definition, at compile time. For instance, adding "-DINT=long" to the CFLAGS variable in the Makefile.inc file to be placed at the root of the source tree will make all SCOTCH\_Num integers become long C integers.

Whenever doing so, make sure to use integer types of equivalent length to declare variables passed to Scotch routines from caller C and Fortran procedures. Also, because of API conflicts, the METS compatibility library will not be usable. It is

usually safer and cleaner to tune your C and Fortran compilers to make them interpret int and INTEGER types as 32 or 64 bit values, than to use the aforementioned flags and coerce type lengths in your own code.

Fortran users also have to take care of another size issue: since there are no pointers in Fortran 77, the Fortran interface of some routines converts pointers to be returned into integer indices with respect to a given array (e.g. see sections 8.6.6, 8.11.4 and 8.16.4). For 32\_64 architectures, such indices can be larger than the size of a regular INTEGER. This is why the indices to be returned are defined by means of a specific integer type, SCOTCH\_Idx. To coerce the length of this index type to 32 or 64 bits, one can use the "-DIDXSIZE32" or "-DIDXSIZE64" flags, respectively, or else use the "-DIDX=" definition, at compile time. For instance, adding "-DIDX="long long" to the CFLAGS variable in the Makefile.inc file to be placed at the root of the source tree will equate all SCOTCH\_Idx integers to C long long integers. By default, when the size of SCOTCH\_Idx is not explicitly defined, it is assumed to be the same as the size of SCOTCH\_Num.

# 10 Examples

This section contains chosen examples destined to show how the programs of the SCOTCH project interoperate and can be combined. It is supposed that the current directory is directory "scotch\_6.0" of the SCOTCH distribution. Character "%" represents the shell prompt.

• Partition source graph brol.grf into 7 parts, and save the result to file /tmp/brol.map.

```
% echo cmplt 7 > /tmp/k7.tgt
% gmap brol.grf /tmp/k7.tgt /tmp/brol.map
```

This can also be done in a single piped command:

```
% echo cmplt 7 | gmap brol.grf - /tmp/brol.map
```

If compressed data handling is enabled, read the graph as a gzip compressed file, and output the mapping as a bzip2 file, on the fly:

```
\% echo cmplt 7 | gmap brol.grf.gz - /tmp/brol.map.bz2
```

• Partition source graph brol.grf into two uneven parts of respective weights  $\frac{4}{11}$  and  $\frac{7}{11}$ , and save the result to file /tmp/brol.map.

```
% echo cmpltw 2 4 7 > /tmp/k2w.tgt
% gmap brol.grf /tmp/k2w.tgt /tmp/brol.map
```

This can also be done in a single piped command:

```
\% echo cmpltw 2 4 7 | gmap brol.grf - /tmp/brol.map
```

If compressed data handling is enabled, use gzip compressed streams on the fly:

```
% echo cmpltw 2 4 7 | gmap brol.grf.gz - /tmp/brol.map.gz
```

• Map a 32 by 32 bidimensional grid source graph onto a 256-node hypercube, and save the result to file /tmp/brol.map.

```
% gmk_m2 32 32 | gmap - tgt/h8.tgt /tmp/brol.map
```

• Build the OPEN INVENTOR file graph.iv that contains the display of a source graph the source and geometry files of which are named graph.grf and graph.xyz.

```
% gout -Mn -Oi graph.grf graph.xyz - graph.iv
```

Although no mapping data is required because of the "-Mn" option, note the presence of the dummy input mapping file name "-", which is needed to specify the output visualization file name.

• Given the source and geometry files graph.grf and graph.xyz of a source graph, map the graph on a 8 by 8 bidimensional mesh and display the mapping result on a color screen by means of the public-domain ghostview PostScript previewer.

```
\% gmap graph.grf tgt/m8x8.tgt | gout graph.grf graph.xyz '-Op{c,f,1}' | ghostview -
```

• Build a 24-node Cube-Connected-Cycles graph target architecture which will be frequently used. Then, map compressed source file graph.grf.gz onto it, and save the result to file /tmp/brol.map.

```
% amk_ccc 3 | acpl - /tmp/ccc3.tgt
% gunzip -c graph.grf.gz | gmap - /tmp/ccc3.tgt /tmp/brol.map
```

To speed up target architecture loading in the future, the decompositiondefined target architecture is compiled by means of acpl.

• Build an architecture graph which is the subgraph of the 8-node de Bruijn graph restricted to vertices labeled 1, 2, 4, 5, 6, map graph graph.grf onto it, and save the result to file /tmp/brol.map.

```
\% (gmk_ub2 3; echo 5 1 2 4 5 6) | amk_grf -L | gmap graph.grf -/tmp/brol.map
```

Note how the two input streams of program amk\_grf (that is, the de Bruijn source graph and the five-elements vertex label list) are concatenated into a single stream to be read from the standard input.

• Compile and link the user application brol.c with the LIBSCOTCH library, using the default error handler.

```
\% cc brol.c -o brol -lscotch -lscotcherr -lm
```

Note that the mathematical library should also be included, after all of the Scotch libraries.

• Recompile a program that used METiS so that it uses Scotch instead.

```
\% cc brol.c -o brol -I${metisdir} -lscotchmetis -lscotch -lscotcherr -lmetis -lm
```

Note that the "-lscotchmetis" option must be placed before the "-lmetis" one, so that routines that are redefined by Scotch are selected instead of their METIS counterpart. When no other METIS routines than the ones redefined by Scotch are used, the "-lmetis" option can be omitted. The "-I\${metisdir}" option may be necessary to provide the path to the original metis.h include file, which contains the prototypes of all of the METIS routines.

# 11 Adding new features to Scotch

Since Scotch is free/libre software, users have the ability to add new features to it. Moreover, as Scotch is intended to be a testbed for new partitioning and ordering algorithms, it has been developed in a very modular way, to ease the development and inclusion of new partitioning and ordering methods to be called within Scotch strategies.

All of the source code for partitioning and ordering methods for graphs and meshes is located in the src/libscotch/ source subdirectory. Source file names have a very regular pattern, based on the internal data structures they handle.

### 11.1 Graphs and meshes

The basic structures in Scotch are the Graph and Mesh structures, which model a simple symmetric graph the definition of which is given in file graph.h, and a simple mesh, in the form of a bipartite graph, the definition of which is given in file mesh.h, respectively. From this structure are derived enriched graph and mesh structures:

- Bgraph, in file bgraph.h: graph with bipartition, that is, edge separation, information attached to it;
- Kgraph, in file kgraph.h: graph with mapping information attached to it;
- Hgraph, in file hgraph.h: graph with halo information attached to it, for computing graph orderings;
- Vgraph, in file vgraph.h: graph with vertex bipartition information attached to it;
- Hmesh, in file hmesh.h: mesh with halo information attached to it, for computing mesh orderings;
- Vmesh, in file vmesh.h: graph with vertex bipartition information attached to it

As version 6.0 of the LIBSCOTCH does not provide mesh mapping capabilities, neither Bmesh nor Kmesh structures have been defined to date, but this work is in progress, and these features should be available in the upcoming releases.

All of the structures are in fact defined as typedefed types.

### 11.2 Methods and partition data

Methods are routines which take one of the above structures as input, and update the fields of the given structure according to the implemented algorithm. Initial methods will behave irrespective of the former values of the structure (like graph growing methods, which compute partitions from scratch), while refinement methods must be provided an existing partition to improve.

In addition to the topological description of the underlying graph, the working graph and mesh structures comprise variables describing the current state of the vertex or edge partition. In all cases is provided a partition array called parttax, of size equal to the number of graph vertices, which tells which part every vertex is assigned to. Other variables comprise the communication load and the load imbalance of the current cut, that is, all of the data necessary to measure the quality of a partition. Some other data are also often provided, such as the number of vertices in each part and the list of frontier vertices. They are not relevant to measure the quality of the partition, but to improve the speed of computations. They are used for instance in the multilevel algorithms to compute incremental updates of the current partition state, without having to recompute these values from scratch by considering all of the graph vertices. Implementers of new methods are highly encouraged to use these variables to speed-up their computations, taking examples on typical algorithms such as the multilevel or Fiduccia-Mattheyses ones.

### 11.3 Adding a new method to Scotch

We will assume in this section that the new method to add is a graph separation method. The procedure explained below is exactly the same for graph bipartitioning, graph mapping, graph ordering, mesh separation, or mesh ordering methods.

Please proceed as explained below.

1. Write the code of the method itself. First, choose a free two-letter code to describe your method, say "xy". In the libscotch source directory, create files vgraph\_separate\_xy.c and vgraph\_separate\_xy.h, basing on existing files such as vgraph\_separate\_gg.c and vgraph\_separate\_gg.h, for instance.

If the method is complex, it can be split across several other files, which will be named vgraph\_separate\_xy\_firstmodulename.c, vgraph\_separate\_xy\_secondmodulename.c, eventually with matching header files.

If the method has parameters, create a structure called VgraphSeparateXy Param, which contains fields of types that can be handled by the strategy parser, such as the INT generic integer type (see below), or double, for instance.

The execution of your method should result in the setting or in the updating of the Vgraph structure that is passed to it. See its definition in vgraph.h and read several simple graph separation methods, such as vgraph\_separate\_zr.c, to figure out what all of its parameters mean.

At the end of your method, always call, when the SCOTCH\_DEBUG\_VGRAPH2 debug flag is set, the vgraphCheck routine, to avoid the spreading of eventual bugs to other parts of the LIBSCOTCH library.

2. Add the method to the parser tables. The files to update are vgraph\_separate\_st.h, where "st" stands for "strategy".

First, edit vgraph\_separate\_st.h. In the VgraphSeparateStMethodType enumeration, add a line for your new method VGRAPHSEPASTMETHXY. Then, edit vgraph\_separate\_st.c, where all of the remaining actions take place.

In the top of the file, add a #include directive to include vgraph\_separate\_xy.h.

If the method has parameters, create a vgraphseparatedefaultxy C union, basing on an existing one, and fill it with the default values of your method parameters.

In the vgraphseparatestmethtab method array, add a line for the new method. To do so, choose a free single-letter code that will be used to designate the new method in strategy strings. If the method has parameters, the last field should be a pointer to the default structure, else it should be set to NULL.

If the method has parameters, update the vgraphseparatestparatab parameter array. Add one data block per parameter. The first field is the name of the method to which the parameter applies, that is, VGRAPHSEPASTMETH XY. The second field is the type of the parameter, which can be:

- STRATPARAMCASE: the support type is an int. It receives the index in the case string, which is provided as the last field of the parameter line, of the given case character;
- STRATPARAMDOUBLE: the support type is a double;
- STRATPARAMINT: the support type is an INT, which is the generic integer type handled internally by Scotch. This type has variable extent, depending on compilation flags, as described in Section 8.1.5;
- STRATPARAMSTRING: a (small) character string;
- STRATPARAMSTRAT: strategy. For instance, the graph ordering method by nested dissection takes a vertex partitioning strategy as one of its parameters, to compute the vertex separators.

The fourth and fifth fields are the address of the location of the default structure and the address of the parameter within this default structure, respectively. From these two values can be computed at run time the offset of the parameter within any instance of the parameter structure, which is used to fill the actual structures in the parsed strategy evaluation tree. The value of the sixth parameter depends on the type of the parameter. It should be NULL for STRATPARAMDOUBLE and STRATPARAMINT parameters, points to the string of available case letters for STRATPARAMCASE parameters, points to the target string buffer for STRATPARAMSTRING parameters, and points to the relevant method parsing table for STRATPARAMSTRAT parameters.

- 3. Edit the makefile of the LIBSCOTCH source directory to enable the compilation and linking of the method. Depending on LIBSCOTCH versions, this makefile is either called Makefile or make\_gen.
- 4. Compile in debug mode and experiment with your routine, by creating strategies that contain its single-letter code.
- 5. To change the default strategy string used by the LIBSCOTCH library, update file library\_graph\_order.c, since it is the graph ordering routine which makes use of graph vertex separation methods to compute separators for the nested dissection ordering method.

## 11.4 Licensing of new methods and of derived works

According to the terms of the CeCILL-C license [6] under which the SCOTCH software package is distributed, the works that are carried out to improve and extend the LIBSCOTCH library must be licensed under the same terms. Basically, it means that you will have to distribute the sources of your new methods, along with the sources of SCOTCH, to any recipient of your modified version of the LIBSCOTCH, and that you grant these recipients the same rights of update and redistribution as the ones that are given to you under the terms of CeCILL-C. Please read it carefully to know what you can do and cannot do with the SCOTCH distribution.

You should have received a copy of the CeCILL-C license along with the SCOTCH distribution; if not, please browse the CeCILL website at http://www.cecill.info/licenses.en.html.

# Credits

I wish to thank all of the following people:

- Patrick Amestoy collaborated to the design of the Halo Approximate Minimum Degree algorithm [48] that had been embedded into Scotch 3.3, and provided versions of his Approximate Minimum Degree algorithm, available since version 3.2, and of his Halo Approximate Minimum Fill algorithm, available since version 3.4. He designed the mesh versions of the approximate minimum degree and approximate minimum fill algorithms, which are available since version 4.0;
- Sébastien Fourestier coded the mapping with fixed vertices, remapping, and remapping with fixed vertices sequential routines that are available since version 6.0;
- Jun-Ho Her coded the graph partitioning with overlap routines that were introduced in the unpublished 5.2 release, and publicly released in version 6.0;
- Alex Pothen kindly provided a version of his Multiple Minimum Degree algorithm, which was embedded into SCOTCH from version 3.2 to version 3.4;
- Luca Scarano, visiting Erasmus student from the *Universitá degli Studi di Bologna*, coded the multilevel graph algorithm in Scotch 3.1;
- Yves Secretan contributed to the MinGW32 port;
- David Sherman proofread version 3.2 of this manual.

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