Minimizing Cache Misses in Scientific Computing Using Isoperimetric Bodies

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A number of known techniques for improving cache performance in scientific computations involve the reordering of the iteration space. Some of these reorderings can be considered coverings of the iteration space with sets having small surface-to-volume ratios. Use of such sets may reduce the number of cache misses in computations of local operators having the iteration space as their domain. First, we derive lower bounds on cache misses that any algorithm must suffer while computing a local operator on a grid. Then, we explore coverings of iteration spaces of structured and unstructured discretization grid operators which allow us to approach these lower bounds. For structured grids we introduce a covering by successive minima tiles based on the interference lattice of the grid. We show that the covering has a small surface-to-volume ratio and present a computer experiment showing actual reduction of the cache misses achieved by using these tiles. For planar unstructured grids we show existence of a covering which reduces the number of cache misses to the level of that of structured grids. Next, we introduce a class of multidimensional grids, called starry grids in this paper. These grids represent an abstraction of unstructured grids used in, for example, molecular simulations and the solution of partial differential equations. We show that starry grids can be covered by sets having a low surface-to-volume ratio and, hence have the same cache efficiency as structured grids. Finally, we present a triangulation of a three-dimensional cube that has the property that any local operator on the corresponding grid must incur a significantly larger number of cache misses than a similar operator on a structured grid.
1 Introduction

A number of known techniques for improving cache performance in scientific computations involve the reordering of the iteration space\(^1\). We present two new methods for partitioning structured grid iteration spaces with minimum-surface cache fitting sets. Such partitionings reduce the number of cache misses to a level that is close to the theoretical minimum. We demonstrate this reduction by actual measurements of cache misses in computations of a second-order stencil operator on structured three-dimensional grids.

A good tiling of the iteration space for structured discretization grids in the presence of limited cache associativity can be constructed by using the interference lattice of the grid. This lattice is a set of grid indices mapped into the same word in the cache or, equivalently, a set of solutions of the Cache Miss Equation \([7]\). In \([2]\) we introduced a (generally skewed) tiling of the iteration space of stencil operators on structured grids with parallelepipeds spanned by a reduced basis of the interference lattice. We showed that for lattices whose second shortest vector is relatively long, the tiling reduces the number of cache misses to a value close to the theoretical lower bound. Constructing the skewed tiling, however, is a nontrivial task, and involves a significant overhead in testing whether a particular point lies inside the tile. Tiling a three-dimensional grid, for example, requires the determination of 29 integer parameters to construct the loop nest of depth six, and involves a significant branching overhead.

We start the paper with deriving lower bounds on the number of cache misses that any algorithm must suffer while computing a local operator on either structured or unstructured grids\(^2\). Subsequently, we introduce two new coverings of structured grids: Voronoi cells and rectilinear parallelepipeds built on the vectors of successive minima of the grid interference lattice. In lattices with a relatively long shortest vector, the cells of both coverings have near-minimal surface-to-volume ratios. Hence, the number of cache misses in the computations tiled with these cells is close to the theoretical minimum derived in \([2]\).

For the computation of local discretization operators on planar, fixed-degree unstructured grids, we construct a near-minimum-perimeter covering by applying the Lipton-Tarjan planar graph separator algorithm \([8]\). The perimeter-to-area ratio of the sets of this covering is \(O(1/\sqrt{S})\), where \(S\) is the cache size. Next, we introduce a class of multidimensional grids, called starry grids, and show that a \(d\)-dimensional starry grid can be covered by sets having a surface-to-volume ratio close to that of structured grids, i.e. \(O(S^{-1/d})\).

Lastly, we construct a fixed-degree unstructured grid that triangulates a three-

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\(^1\)In \([4]\) we laid the foundation for the study of reorderings to improve cache performance of local operators on structured grids. We extend those results in this paper to the construction of practical, near-optimal tilings of structured grids, and to the study of cache misses for local operators on unstructured grids.

\(^2\)The derivation is a simplification of the proof given in \([4]\) for structured grids and extends its application to unstructured grids.
dimensional cube and show that the grid can not be covered with sets having small surface-to-volume ratios. The last result shows that any computation of a local operator on such a three-dimensional grid must suffer a larger number of cache misses than the computation of a similar operator on a structured grid of the same size. Hence, general unstructured grids of dimension higher than two are provably less efficient in a cache utilization than structured grids.

2 Cache and Discrete Geometry

Local operators on grids. We consider the problem of computing array \( q \) by applying a local discretization operator \( K \) to array \( u \) (i.e. \( q = Ku \)) defined at the vertices of an undirected graph \( G = (V, E) \). Locality of \( K \) means that computation of \( q(x) \), \( x \in V \), involves values of \( u(y) \), \( y \in V \), where \( y \) is at a (graph) distance at most \( r \) from \( x \). This \( r \) is called the order of \( K \) and is assumed to be independent of \( G \). Arrays \( q \) and \( u \) are distinct. Hence, the values of \( q \) can be computed in arbitrary order.

We consider structured and unstructured grids that have an explicit or implicit embedding into Euclidean space. Structured grids can be defined as Cartesian products of line graphs, while edges of unstructured grids are defined explicitly, for example by an adjacency matrix. We assume that the maximum vertex degree is independent of the total number of vertices. A grid is called planar if its vertices and edges can be embedded into a plane without edge intersections. A grid is called a triangulation of a body \( B \) if it can be represented as a one-dimensional skeleton of a simplicial partition of \( B \) (see \[4\]).

Cache Model. We consider a single-level, virtual-address-mapped, set-associative data cache memory, see \[3\]. The memory, with a total capacity of \( S \) words, is organized in \( z \) sets of \( a \) (associativity) lines each. Each line contains \( w \) words. Hence, the cache can be characterized by the parameter triplet \((a, w, S)\), and its size \( S \) equals \( a \times z \times w \) words. A cache with parameters \((S/w, w, S)\) is called fully associative, and a cache with parameters \((1, w, S)\) is called direct-mapped.

The cache memory is used as a temporary fast storage of words used for processing. A word at virtual address \( A \) is fetched into cache location \((a(A), z(A), w(A))\), where \( w(A) = A \mod w \), \( z(A) = (A/w) \mod z \), and \( a(A) \) is determined according to a replacement policy (usually a variation of least recently used). The replacement policy is not important within the scope of this paper since our lower bounds are valid for any replacement policy and our upper bounds hold even for a direct mapped cache.

The number of cache misses incurred in computation of \( q \) depends on the order in which elements of \( u \) are stored in the main memory. We assume that for structured grids an element \( u(i_1, \ldots, i_d) \) is stored at address \( A = i_1 + n_1 i_2 + n_1 n_2 i_3 + \cdots + n_1 \cdot \ldots \cdot n_{d-1} i_d \), where \( n_1, \ldots, n_{d-1} \) are the grid sizes. For unstructured grids we don’t assume any particular ordering in memory of the grid points (and, hence, of unstructured grids we don’t assume any particular ordering in memory of the grid points (and, hence, of
elements of \( u \)). Instead, we choose an ordering that reduces the number of cache misses.

**Replacement loads.** A **cache miss** is defined as a request for a word of data that is not present in the cache at the time of the request. A **cache load** is defined as an explicit request for a word of data for which no explicit request has been made previously (a **cold load**), or whose residence in the cache has expired because of a cache load of another word of data into the exact same location in the cache (a **replacement load**). Cache load is used as a technical term for making some formulas and their proofs shorter. The definitions of cold and replacement loads are analogous to those of cold and replacement cache misses \[7\], respectively, and if \( w \) equals 1 they completely coincide.

**Isoperimetric Sets.** In addition to inevitable cold loads, some replacement loads must occur, as formalized in Lemma \[1\], because some values have to be dropped from cache before they are fully utilized. This leads us to a lower bound on cache misses, see Theorems \[2\]. This bound includes the surface-to-volume ratio of isoperimetric subsets of the grid, that is, sets whose boundary size is \( 3S \) and that have maximum volume.

**Surface-to-volume ratio.** Some replacement loads may be avoided by careful scheduling of the computations. One technique for minimizing the number of replacement loads is to cover the grid \( G \) with conflict-free sets \( V_i (V = \bigcup_{i=1}^{k} V_i, |V_i| = S) \), that is, sets whose vertices are all mapped to different locations in cache. If we calculate \( q \) in all vertices of \( V_i \) before calculating it in vertices of \( V_j, j = i+1, \ldots, k \), a replacement load can occur only at vertices having neighbors in at least two sets (boundary vertices). We consider only bounded-degree graphs, so if we can find a covering with sets \( V_i \) having volumes \( |V_i| \) close to \( S \) and a minimal number of boundary vertices \( |\partial V_i| \) (and boundary edges) i.e., bodies with minimum surface-to-volume ratio, then the computation of \( q \) will incur a number of replacement loads close to the minimum. On the other hand, the total partition boundary \( \sum_{i=1}^{k} |\partial V_i| \) can be used to obtain a lower bound on the number of replacement loads, see section \[3\], cf. \[4\]. Deviating from the literal meaning of the word “isoperimetric” and following common practice, we call sets having the minimum number of boundary points for a given number of total points also isoperimetric.

### 3 A lower bound on cache misses for local operators

In this section we consider the following problem: for a given grid \( G \) and a local operator \( K \), how many cache misses must be incurred in order to compute \( q = Ku \), where \( q \) and \( u \) are two distinct arrays defined on the grid. We provide a lower bound on the number of cache misses in any algorithm, regardless of the order in which the grid points are visited during the computation of \( q \). The lower bound contains the surface-to-volume ratio of isoperimetric sets of the grid. This ratio can be well estimated for structured grids, and for FFT grids, to be described in Section \[5.3\]. It may be shown that our lower bound is tight for the above-mentioned grids, and in general for any grid which may be covered by sets of size \( S \) having an optimal surface-to-volume ratio.
We use the following terminology to describe the operator $K$. Locality of $K$ means that the value of $q$ at grid point $x$ is a function of the values $u(y)$, where $y$ is a grid point at a graph distance at most $r$ from $x$ ($r$ is called the radius, or order, of $K$). We call an operator of radius $r$ symmetric if it uses values of $u$ at all grid points within distance $r$ from the target point. In this section we obtain a lower bound for a symmetric operator of unit radius, which obviously is a lower bound for symmetric operators of larger radii as well.

### 3.1 Pointwise Computations

Depending on the separability of the local operator, it has to be computed pointwise, or it may allow computation in edgewise fashion. If an operator is not separable, it requires values of $u$ at all neighbor points simultaneously to compute a value of $q$. We call such computation pointwise. In this subsection we assume that computation of $q$ on the grid $G$ is performed in a pointwise fashion, that is, at any grid point the value of $q$ is computed completely before computation of the value of $q$ at another point is started. Separable operators, which can be evaluated edgewise, are considered in the next section.

In order to compute the value of $q$ at a grid point $x$, the values of $u$ at the neighbor points of $x$ must be loaded into the cache (points $y$ and $x$ are neighbors if they are connected by a grid edge). If $x$ is a neighbor of $y$ and $u(y)$ has been loaded in cache to compute $q(z)$ but is dropped from the cache before $q(x)$ is computed, then $u(y)$ must be reloaded, resulting in a replacement load. Our lower bound on cache loads is based on the following simple observation.

**Lemma 1.** Let values of $u$ at a vertex set $X$ first be used for computation of $q$ in a vertex set $U_0$, and next for computation of $q$ in a vertex set $U_1$, $U_0 \cap U_1 = \emptyset$. This computation incurs at least $|X| - S$ replacement loads.

**Proof.** Since the cache can hold at most $S$ values, at least $|X| - S$ values must have been dropped from the cache by the time computations at the points of $U_0$ are done. Since all values at points of $X$ are necessary for computing values at $U_1$, they have to be reloaded into the cache. Hence, computations of values at points of $U_1$ will result in at least $|X| - S$ replacement loads. \[\square\]

To estimate for a given algorithm the number of elements, $\rho$, of array $u$ that must be replaced, we partition $V$ into a disjoint union of $k$ sets $V_i$, with $V = \bigcup_{i=1}^{k} V_i$, in such a way that $q$ is computed at all points of $V_i$ before it is computed at any point of $V_{i+1}$, see Figure 1. Let $B_i^l$ and $B_i^u$ be (possibly overlapping) subsets of $V_i$ which have neighbors in $\bigcup_{j<i} V_j$ and $\bigcup_{j>i} V_j$, respectively. The set $B_i = B_i^l \cup B_i^u$ is the boundary of $V_i$.

Replacement loads of values at the points of $V_i$ will be incurred when such points show up as neighbors in other vertex sets. We apply Lemma 1 to the two pairs of sets in which boundary points of $V_i$ occur as members and neighbors:

$$\bigcup_{j<i} V_j \text{ and } V_i$$
Figure 1. Iteration space $V$ is partitioned in a sequence of regions $V_i$. Reloading of some values of $u$ on the boundary of $V_3$ (heavy and dotted lines, corresponding to $|B_i^u|$ and $|B_i^B|$, respectively) results in at least $|B_i^l| + |B_i^u| - 2S$ cache loads.

$V_i$ and $\cup_{j>i} V_j$

This gives us the following bounds on replacement loads:

$\rho_i^l \geq |B_i^l| - S$

and

$\rho_i^u \geq |B_i^u| - S,$

respectively. Hence, in each set of the partition at least $\rho_i$ values have to be reloaded (see Figure 1), with

$\rho_i = \rho_i^l + \rho_i^u \geq |B_i^l| + |B_i^u| - 2S \geq |B_i| - 2S.$

The total number of reloaded values in the course of computing $q$ on the entire grid will be at least $\rho = \sum_{i=1}^{k} \rho_i$, for which we have the following bound:

$\rho \geq \sum_{i=1}^{k} \rho_i \geq \sum_{i=1}^{k} |B_i| - 2kS.$
Let $v$ be the maximum number of points in a set with $3S$ points on its boundary, i.e., let $v$ be the number of points in an isoperimetric set with $3S$ boundary points. Choosing a partition $V = \bigcup_{i=1}^{k} V_i$ in such a way that $|V_i| = v$, we have $|B_i| \geq 3S$, hence

$$\rho \geq S\frac{|V|}{v}. \hspace{1cm} (1)$$

Thus we have the following result.

**Theorem 2.** The number of cache misses $\mu$ in the evaluation of a symmetric operator on a grid $G = (V, E)$ is bounded as follows:

$$\mu \geq \frac{1}{w}(|V| + \rho) \geq \frac{1}{w}|V|(1 + \frac{1}{3}\alpha(G))$$

where $\alpha(G)$ is the surface-to-volume ratio of isoperimetric subsets of $V$ with $3S$ boundary points.

**Proof.** We sum the number of replacements in (1) with the number of cold loads $|V|$ and notice that $\frac{v}{w} = 1/3\alpha(G)$. Then we notice that any cache miss results in a load of $w$ words into the cache, and that in the best possible case all $w$ words contain useful data. \[\square\]

### 3.2 Edgewise Computations

The pointwise calculation model used in the previous subsection is too restrictive in many cases. Using separability of the operator, the number of cache misses may be reduced. In this section we present lower bounds for more general computations where values of $q$ may be updated multiple times in arbitrary order. We call these computations edgewise.

An edgewise computation is performed at the vertices of a bipartite graph $H = (V^I, V^O, E)$ where, $V^I$ and $V^O$ are vertex sets, both equal to $V$, and $(x, y), x \in V^I, y \in V^O,$ is an edge in $H$ iff $x$ and $y$ are neighbors in $G$ or $x = y$. The values of $u$ are given in the nodes of $V^I$, and values of $q$ have to be computed at the nodes of $V^O$. An atomic step in an edgewise computation is the evaluation of a function of two variables corresponding to an edge of $H$. If a value at an end point of the edge is currently not loaded, then the computation suffers a cache load. All edges of the grid must be visited. We want to estimate the number of cache loads that each computation of $q = Ku$ must suffer.

The arguments in the proof of the lower bound of Theorem 2 can be modified by partitioning the edges of $H$ into disjoint sets $E_i$, with $E = \bigcup_{i=1}^{k} E_i$, in such a way that processing of any edge in $E_i$ precedes processing of any edge in $E_{i+1}$, and such that the size of boundary of $E_i$ is at least $3S$. Here the boundary of an edge set $E_i$ is the set of vertices shared by an edge in $E_i$ and an edge not in $E_i$. The surface-to-volume ratio of an edge set is the ratio of its number of boundary vertices to the number of its edges. We define $\beta(G)$ to be the minimum surface-to-volume
ratio of the edge sets in $H$ (derived from $G$) having a boundary of size $3S$. In other words $\beta(G)$ is the number of boundary points divided by the number of edges in isoperimetric sets in $H$ having $3S$ boundary points. The following result can be proved using arguments completely analogous to those in Theorem 2.

**Theorem 3.** The number of cache misses in a calculation of a separable symmetric operator on a grid $G = (V, E)$ is bounded as follows:

$$\mu \geq \frac{1}{w} |E|(1 + \frac{1}{3} \beta(G))$$

where $\beta(G)$ is the minimum of the surface-to-volume ratio over subsets of $E$ with $3S$ boundary points.

### 4 Structured Grids

#### 4.1 Interference Lattice

*Interference lattice.* Let $u$ be a $d$-dimensional array defined at the vertices of a structured $d$-dimensional grid of size $n_1 \times \cdots \times n_d$. Let $L$ be a set in the index space of $u$ having the same image in cache as the index $(0, \ldots, 0)$. $L$ is a lattice in the sense that there is a generating set of vectors $\{b_i\}$, $i = 1, \ldots, d$, such that $L$ is the set of grid points $\{\sum_{i=1}^{d} x_i b_i \mid x_i \in \mathbb{Z}\}$. We call $L$ the *interference lattice* of $u$. For a direct-mapped cache it can be defined as the set of all vectors $(i_1, \ldots, i_d)$ that satisfy the Cache Miss Equation:

$$(i_1 + n_1 i_2 + n_1 n_2 i_3 + \cdots + n_1 \cdots n_{d-1} i_d) \mod S = 0.$$  

We will use some geometrical properties of lattices. Let $B$ be a convex body of volume $V$, symmetrical about the origin. The minimal positive $\lambda_i$ such that $\lambda_i B$ contains $i$ linearly independent vectors of $L$ is called the $i^{th}$ successive minimum vector of a lattice $L$ relative to $B$. A theorem by Minkowski, see [1] (Ch. VIII, Th. V), asserts that

$$\frac{2d}{dV} \leq \Pi_{i=1}^{d} \lambda_i \det L \leq \frac{2d}{V}.$$  

Note that the ratios of lattice successive minima relative to the unit cube and to the unit ball can be bounded: $1/d \leq \lambda_i^{cube}/\lambda_i^{ball} \leq d$. We use successive minima relative to the unit ball and the unit cube in the Sections 4.2 and 4.3 respectively. In both cases we call $f = \lambda_d/\lambda_1$ the *eccentricity* of the lattice (not to be confused with eccentricity of a reduced basis, defined in [3], Section 4). The eccentricities relative to a ball and a cube may differ by a factor of $d^2$ at most.

In [3] we introduced a tiling by parallelepipeds built on a reduced basis of the interference lattice which decreases the number of the cache misses to a level close to the theoretical lower bound that we also derived. Measurement shows that this tiling incurs significantly fewer cache misses than a compiler-optimized code with canonical loop ordering. However, it has a high computational cost, since it
depends on a significant number of integer parameters, and its implementation scans a substantial number of the grid points to select those suitable for cache conflict-free computations. This prompts us to consider alternative tilings, specifically with Voronoi cells and with successive minima parallelepipeds. We show that these tilings have good surface-to-volume ratios if the lattice eccentricity is small.

4.2 Voronoi Tiling

A Voronoi tiling is a tiling of the grid by completed cells $C$ (Voronoi tile) of the Voronoi diagram of the interference lattice. For each lattice point $x$ a Voronoi cell is the set of points which are closer to $x$ than to any other lattice point. All integer points inside each Voronoi cell are mapped into the cache without conflicts. Voronoi cells may not form a tiling since some integer points can be located on a cell boundary. There are many qualitatively equivalent ways to complete the cells to form a tiling. One way is to choose a basis in the space of the lattice and assign an integer point to the cell whose center is lexicographically closest to the point.

In order to estimate the surface-to-volume ratio of a Voronoi cell $C$ we note that the completed Voronoi cells form a tiling of space. Hence, the volume of $C$ equals the determinant of the lattice (defined by (2)), which is equal to $S$, see [2]. On the other hand, let $C_o$ be a Voronoi cell centered at $o$. Each vertex $v$ of $C_o$ is equidistant from $d$ lattice points. Let $r$ be that distance, which will in general be different for different $v$. According to the definition of the Voronoi cell, the ball of radius $r$, centered at $v$, contains no other lattice points. Hence $r \leq R$, where $R$ is the radius of a maximal ball of the lattice (a lattice-points-free ball of maximal radius). Hence, $C_o$ is contained in a ball of radius $R$, centered at $o$. Thus, the surface area of $C_o$ is bounded by the surface of a ball of radius $R$, which equals $dV_d R^{d-1}$, where $V_d = \frac{\pi^{d/2}}{\Gamma(1+d/2)}$ is the volume of the unit $d$-dimensional ball (see [1] Ch. IX.7).

We estimate the radius of the maximal ball $R$ by induction on the dimension of a sublattice. Let $R_i$ be the radius of the maximal ball inscribed into the lattice $L_i$ generated by the first $i$ minima vectors $v_i$ of $L$ relative to the $i$-dimensional ball. Then we have (see Figure 3):

$$R_i^2 \leq (h_i/2)^2 + R_{i-1}^2 \leq (\lambda_i/2)^2 + R_{i-1}^2,$$

where $h_i$ is the distance between hyperplanes spanned by $L_{i-1}$ and $L_{i-1} + v_i$, respectively, and $\lambda_i$ is the $i^{th}$ successive minimum. Induction on $i$ gives the following result.

**Lemma 4.** The following relation holds for the radius of a lattice-points-free ball in a $d$-dimensional lattice $L$:

$$R^2 \leq \frac{1}{4} \sum_{i=1}^{d} \lambda_i^2. \quad (4)$$

where $\lambda_1 \leq \cdots \leq \lambda_d$ are successive minima of $L$. 
Figure 2. Let $L_i$ be a lattice generated by the first $i$ minima vectors of $L$. An intersection of a maximal ball of $L_i$ with the subspace of $L_{i-1}$ is contained in a maximal ball of $L_{i-1}$. Hence $R_i^2 \leq (h_i/2)^2 + R_{i-1}^2$ where $h_i$ is the distance between subspaces $L_{i-1}$ and $v_i + L_{i-1}$.

Since $C$ is contained in a ball of radius $R$ and both $C$ and ball are convex bodies, the surface area $A$ of $C$ does not exceed the surface area of the ball and we have an estimation

$$A(C) \leq dV_dR^{d-1} \leq d(\sqrt{d}/2)^{d-1}V_d\lambda_d^{d-1} \leq d^{d+1}/d^{1/d} f^{(d-1)^2/d} \lambda_{d-1}/d,$$

where we used the estimation $\lambda_d^d \leq \frac{d^d}{d^d} f^{d-1} S$ derived from (3), and the bound $R \leq \sqrt{\frac{d}{2}} \lambda_d$ which follows from (4). This implies the following result.

**Theorem 5.** The surface-to-volume ratio of a lattice Voronoi cell $C$ can be estimated as:

$$\frac{A(C)}{V(C)} \leq c_d f^{(d-1)^2/d} S^{-1/d},$$

where $c_d$ is a constant depending on $d$ only, and $f$ is the lattice eccentricity.

### 4.3 Successive Minima Tiling

The Voronoi cell tiling has cache-conflict-free tiles of maximum possible volume $S$, and of small surface-to-volume ratio. However, the tiles may have many faces, and it may be computationally expensive to traverse the grid points inside a tile. It is more desirable to use rectangular tiles. A *successive minima tiling* is a tiling by Cartesian blocks constructed using successive minima lattice vectors of the unit cube. Such a block $Q$ can be described by the system

$$|x_i| \leq b_i, \quad i = 1, \ldots, d, \quad \lambda_1 \leq b_i \leq \lambda_d.$$  

where $\lambda_1 \leq b_i \leq \lambda_d$.

The block $Q$ can be constructed by the following “inflating” process. Take an initial cube of the form (4), with $b_i = 1, \quad i = 1, \ldots, d$, and increment all $b_i$ equally.
until the face $x_i = b_i$ contains a lattice point. Continue to increment values of all $b_j$ for which the face $x_j = b_j$ has no lattice points. At the end we obtain a block of the form $(\mathcal{F})$, containing a lattice point on each of its faces and containing no lattice points inside except $o$. If each successive minimum vector has end points in distinct faces of the block, then $b_i = \lambda_i$ (after an appropriate reordering of the coordinates).

On the other hand, it is not difficult to construct a three-dimensional lattice such that the block satisfies $b_1 = \lambda_1$, $b_2 = b_3 = \lambda_2 < \lambda_3$, in which case the volume of the block would be strictly less than $\lambda_1 \cdots \lambda_d$.

Any translation of the block $Q' = \frac{1}{2}Q$ obviously contains at most one lattice point and can be used for conflict-free tiling. This block has a low surface-to-volume ratio if the lattice has bounded eccentricity, which can be seen from the following inequalities: $A(Q') \leq 2d\lambda_d^{d-1}$ and $V(Q') \geq \lambda_1^d$. Since $\lambda_1 = \frac{\lambda}{f} \geq \frac{2}{\sqrt{dV_d}}^{1/d}$, as follows from $(\mathcal{F})$, we obtain the following result.

Theorem 6. The surface-to-volume ratio of the block $Q'$ obtained in a successive minima procedure can be estimated as follows:

$$\frac{A(Q')}{V(Q')} \leq 2d\lambda_1^{d-1}/\lambda_1 \leq d(dV_d)^{1/d} f^{-1/d},$$

where $V_d$ is a constant depending on $d$ only, and $f$ is the lattice eccentricity.

"Figure 3. Comparison of measured cache misses for the second order stencil operator as a function of the first grid dimension ($40 \leq nx \leq 99$, $ny = 97$, $nz = 99$). The top curve shows the number of cache misses for the compiler optimized canonically ordered nest. The bottom curve is obtained for tilings with successive-minima parallelepipeds."

As a representative example, the number of measured primary cache misses for tilings of three-dimensional grids of sizes $40 \leq nx \leq 99$, $ny = 97$, $nz = 99$ with
successive minima parallelepipeds is shown in Figure 3. The computation evaluates a linear operator on the standard 13-point star stencil. Experiments were performed on an SGI Origin 2000 machine with a MIPS R10000 processor.

It is easy to show that the lattice eccentricities \( f \) can be bounded by the eccentricity of a reduced basis as defined in [2], times a constant depending on \( d \) only. Hence, it follows from Theorems 5 and 6 that the Voronoi and successive minima tilings have the same asymptotic surface-to-volume ratio—and therefore the same cache efficiency—as the tiling with fundamental parallelepipeds derived in [2].

5 Unstructured Grids

5.1 Lipton-Tarjan Covering

In this section we present a covering of a planar bounded-degree grid with vertex sets of size at most \( S \) that have an average surface-to-volume ratio equal to \( O(1/\sqrt{S}) \). The covering can be used for computing a first-order operator on a \(|V|\)-vertex planar grid with \( O(|V|/\sqrt{S}) \) replacement loads. The covering is based on the Lipton-Tarjan separator theorem, which asserts that any planar graph of \(|V|\) vertices has a vertex separator of size \( O(\sqrt{|V|}) \). The separator can be constructed in \( O(|V|) \) time [8].

We consider bounded-degree unstructured grids, that is, grids having fixed maximum vertex degree \( d \), independent of the grid size. (Calculation on unbounded-vertex-degree grids may cause approximation problems and numerical instability. Consequently, most numerical methods employ bounded-degree grids.) For bounded degree grids a node cut of size \( O(|V|) \) has a corresponding edge cut of size \( O(|V|) \), and vice versa. Hence, the Lipton-Tarjan separator theorem (see [8], section 2, Corollary 2) can be reformulated as follows: By removing \( O(\sqrt{|V|}) \) edges from a \(|V|\)-vertex bounded-degree planar graph it can be separated into connected disjoint subgraphs, each having at most \( 2|V|/3 \) vertices.

We construct the covering by applying the Lipton-Tarjan theorem recursively. First, we choose an edge cut \( C \) of the original graph \( G = (V, E) \), such that \( |C| \leq c_0 \sqrt{|V|} \), where \( c_0 \) is independent of \(|V|\). According to the Lipton-Tarjan separator theorem, the cut can be chosen in such a way that it will split the graph into connected components \( G_i = (V_i, E_i), \quad i = 1, \ldots, k, \quad |V_i| \leq 2|V|/3 \). Adding an extra step in this partition, we can assume that \( |V_i| \leq |V|/2 \) while \( |C| \leq c_1 \sqrt{|V|} \) for a bigger constant \( c_1 \). Then, we recursively bisect each connected component \( G_i = (V_i, E_i) \) while \( |V_i| > S \). We call this covering a Lipton-Tarjan covering.

This partition process can be represented by a cut tree \( T \) whose nodes are partitioned connected components of the grid. The tree will be used to estimate the total number of removed edges to construct a Lipton-Tarjan covering. Let a connected component \( C \), represented by node \( t \) of \( T \), be split into components \( C_1, \ldots, C_m \) by a Lipton-Tarjan cut. We draw an edge between \( t \) and each of its child nodes representing \( C_1, \ldots, C_m \). However, we do not include in \( T \) the connected components of size smaller than \( S \). Hence, the size of each leaf (i.e. a node having no children) exceeds \( S \). Connected components smaller than \( S \) do not contain any cut edges and they are not needed for the estimate. To each node \( t \) of \( T \) we assign
size $s(t)$, which equals the number of vertices in the set represented by $t$, and weight $w(t) = \sqrt{s(t)}$.

**Lemma 7.** The total number of edges in all cuts of a Lipton-Tarjan covering is $O(\sqrt{|V|})$.

**Proof.** The total number of edges in all cuts made to construct a Lipton-Tarjan covering can be bounded by $O(\sigma(T))$, where

$$\sigma(T) = \sum_{t \text{ node of } T} w(t)$$  \hspace{1cm} (6)

We use two properties of the weights. First,

$$\sum_{l \text{ leaf of } T} w(l) \leq |V|/\sqrt{S},$$  \hspace{1cm} (7)

since the maximum of the $\sum \sqrt{s(l)}$, subject to $\sum s(l) = |V|$ and $s(l) \geq S + 1$, is attained for $s(l) = S + 1$ for all $l$. Second, for each node $t$ of $T$ we have

$$w(t) < 1/\sqrt{2} \sum_{\tau \text{ child of } t} w(\tau),$$  \hspace{1cm} (8)

which follows from Proposition 10 with $d = 2$, see Appendix.

Now $\sigma(T)$ can be estimated in two steps. First, we replace weights in each nonleaf $t$ by the right hand side of (8), going bottom up from the leaves to the root of $T$. This operation will not decrease the total weight. Second, we carry summation of new weights across nodes of $T$ by noticing that each leaf $l$ deposits into $\sigma(T)$ a weight of at most

$$w(l)(1 + 1/\sqrt{2} + 1/\sqrt{2^2} + \ldots) \leq w(l)(2 + \sqrt{2}).$$

Hence, it follows from (7) that

$$\sigma(T) \leq (2 + \sqrt{2})|V|/\sqrt{S},$$  \hspace{1cm} (9)

so the total number of edges in all cuts is $O(|V|/\sqrt{S})$. \hfill \Box

Now we prove the main result of this section. From a lower bound on the number of replacement loads for computations of star stencil operators on structured two-dimensional grids, see Section 3, cf. [2], it follows that the order of this bound can not be improved.

**Theorem 8.** Any first-order operator $K$ on a bounded-degree planar grid $G = (V,E)$ can be computed with $O(|V|/\sqrt{S})$ replacement loads.

**Proof.** First, we reorder vertices of the grid in such a way that vertices of each set of the Lipton-Tarjan covering will occupy contiguous memory locations. Then
we compute $K$ on each set, one at a time. In this computation replacement loads can happen only at the vertices of the cuts of the grid. According to Lemma 7 the number of such vertices does not exceed $O(|V|/\sqrt{S})$.

5.2 Covering of Starry Grids

In the previous sections we showed that structured and planar grids can be covered by sets having low surface-to-volume ratios. That implies that local operators of fixed order on such grids can be evaluated with high efficiency of cache utilization. In this section we introduce a class of multi-dimensional unstructured grids, which we call starry grids. We show that cache efficiency of starry grids is the same as that of structured grids.

Definition 9. We call a grid a $d$-dimensional starry grid if it can be mapped to a grid in $d$-dimensional Euclidean space that has the following two properties:

- The ratio of the length $L$ of the longest edge of the grid to the length $l$ of the shortest edge of the grid is limited by a constant independent of the number of grid points:

$$L \leq c_0 l.$$  

(10)

- There are no grid points at a distance shorter than $l$.

A vertex of a starry grid can be adjacent only to grid points contained in a ball of radius $L$ centered at this point. On the other hand, a ball of radius $l$ around any vertex of a starry grid is free of other grid points. Hence, the vertex degree of a $d$-dimensional starry grid is bounded by a constant depending on $d$ only. Another property of starry grids is that any subgrid is starry as well. Any grid with $|V|$ vertices is a $(|V|−1)$-dimensional starry grid, since it can be mapped onto the vertices of a unit $(|V|−1)$-dimensional simplex. In this paper, however, we consider $d$ to be fixed, and $|V|$ to be a parameter.

Starry grids are common in many computations, such as those involving particles distributed in a finite domain and interacting via a short range potential. Unstructured discretization grids for solving partial differential equations are often starry as well. While there is no obvious way to verify that an arbitrary grid is a $d$-dimensional starry grid, starriness of a grid embedded into Euclidean space can easily be verified. One simple way to construct a starry grid is to delete some vertices and their incident edges from a structured grid.

We will show that a $d$-dimensional starry grid $G = (V, E)$ can be covered by sets of size $S$ having at most $c|V|S^{-\frac{1}{2}}$ boundary points in total, see Theorem 12. This covering, as in the case of planar grids, is based on a cutting theorem, specifically, the Hyperplane Cut Theorem (Theorem 11), asserting that there is a hyperplane bisecting $V$ into almost equal sized parts while cutting at most $c|V|S^{-\frac{1}{2}}$ edges of the grid. From this we deduce the main result of the section.
Theorem 10. Any first-order operator \( K \) on a starry \( d \)-dimensional grid \( G = (V, E) \) can be computed with \( O(|V|S^{-\frac{1}{2}}) \) replacement loads.

Proof. First, we reorder vertices of the grid in such a way that the vertices of each set of the covering occupy contiguous memory locations. Then we compute \( K \) within each set separately. In this computation replacement loads can happen only at the vertices of the cuts of the grid. According to Theorem 12 the number of such vertices does not exceed \( O(|V|S^{-\frac{1}{2}}) \).

From a lower bound on the number of replacement loads for computations of operators on structured \( d \)-dimensional grids, see Section 3, it follows that this bound can not be improved.

It is not difficult to see that any continuous convex body has a small bisector (for example, a hyperplane orthogonal to a diameter of the body). It is not surprising, then, that if a grid represents the body well, it has a small bisector size as well. We will construct a set containing \( 3d \) vectors, and show that the bisecting hyperplane can be chosen to be normal to one of these vectors. This constitutes an algorithm of complexity \( O(|V|^2) \) for finding such a bisector.

The following is a multi-dimensional analog of the Lipton-Tarjan cut theorem.

Theorem 11. (Hyperplane Cut Theorem) For any starry \( d \)-dimensional grid \( G = (V, E) \) there is a hyperplane cut of size \( O(|V|^d) \) separating vertices of the grid into two sets of size at least \( |V|/3 \).

Proof. Let us consider vectors of unit length \( u_i \in \mathbb{R}^d, |u_i| = 1, i = 1, \ldots, k \) such that all vertices have different orthogonal projections onto each \( u_i \). Then we choose slabs \( S_i \) bounded by hyperplanes orthogonal to \( u_i \) : \( S_i = \{ x \in \mathbb{R}^d | \lambda_i \leq u_i \cdot x \leq \mu_i \} \), trisecting \( V \), see Figure 4, that is

\[
|\{ v \in V | u_i \cdot v \leq \lambda_i \}| \geq |V|/3 \quad \text{while} \quad |\{ v \in V | u_i \cdot v < \lambda_i \}| < |V|/3, \tag{11}
\]

\[
|\{ v \in V | u_i \cdot v \geq \mu_i \}| \geq |V|/3 \quad \text{while} \quad |\{ v \in V | u_i \cdot v > \mu_i \}| < |V|/3.
\]

meaning that each slab contains at least \( |V|/3 \) points, while at most \( |V|/3 \) grid points can be contained strictly inside a slab. We will show that \( u_1, \ldots, u_k \) can be chosen in such a way that at least one slab is wide, that is \( h_i = \mu_i - \lambda_i \geq O(|V|^{1/d}) \).

If \( |V| \) is big enough, then it follows from (10) that no grid edge can pierce this slab, hence there exists a hyperplane \( H_i = \{ x : u_i \cdot x = \eta_i \}, \lambda_i < \eta_i < \mu_i \) that intersects at most \( O(|V|^{\frac{d-1}{2}}) \) grid edges. This hyperplane separates grid points into sets containing at least \( |V|/3 \) points.

Let \( V^i \) be the set of grid points contained in exactly \( i \) slabs, and let \( V^j_j \) be the subset of \( V^i \) contained in \( S_j \). Since \( V^i, i = 1, \ldots, k \), are disjoint sets and \( \cup_{i=1}^k V^i \subseteq V \), we have

\[
\sum |V^i| \leq |V|. \tag{12}
\]
Figure 4. Finding a wide bisecting slab. $V^2$ is the set of points contained in the thick-lined polygons, minus those contained in $V^3$, the shaded polygon.

Since each slab contains at least $|V|/3$ grid points, it follows that

$$\sum_j |V^j_i| \geq |V|/3.$$ 

If we sum all points in all slabs, then each point in $V^i$ will be counted exactly $i$ times, hence

$$\sum_{1 \leq i \leq k} i|V^i| \geq \frac{k}{3}|V|,$$

and

$$\sum_{i \geq d} i|V^i| \geq \frac{k}{3}|V| - \sum_{i < d} i|V^i| \geq \left(\frac{k}{3} - d + 1\right)|V|,$$ (13)

where the last inequality follows from (12). Let $P_I$, $I = \{i_1, \ldots, i_d\}, 1 \leq i_1 < \cdots < i_d \leq k$, be a parallelepiped formed by the intersection of $d$ different slabs. Obviously, $\cup_{i \geq d} V^i \subseteq \cup_I P_I$. Let $U_I$ be the number of grid points in $P_I$, then

$$\sum_I U_I \geq \sum_{i \geq d} \binom{i}{d} |V^i| \geq 1/d \sum_{i \geq d} i|V^i|.$$ 

If we now choose $k = 3d$, it follows from (13) that

$$\sum_I U_I \geq \frac{1}{d}|V|.$$ (14)
According to the second property of starry grids, the balls \( B_l \) of radius \( l \), centered at the grid points, do not intersect, so
\[
\sum_I U_I \leq (c_3 l^d)^{-1} \sum_I \text{vol}(P_I + B_l), \tag{15}
\]
where \( c_3 l^d = \text{vol}(B_l) \).

Now we exercise our freedom to select the vectors \( u_i \). We choose them to be the rows (normalized to unit length) of a \( 3d \times d \) generalized Vandermonde matrix
\[
W = \{(i - \alpha)^j, \ i = 1, \ldots, 3d, \ j = 0, \ldots, d - 1, \ 0 < \alpha < 1\}
\]
and choose \( \alpha \) in such a way that \( u_i(v_P - v_Q) \neq 0 \), where \( v_P, v_Q \) are different grid points. These gives us at most \( 3d|V|^2 \) nontrivial constraints. We choose \( \alpha \) such that inequality holds for all of them. Then each parallelepiped \( P_I \) may be described by a system of inequalities
\[
-h_I \leq D_I W_I (x - x_I) \leq h_I,
\]
where \( W_I \) is a square matrix, consisting of rows \( (i_1, \ldots, i_d) \) of \( W \), and \( h_I = (h_{i_1}, \ldots, h_{i_d})^t \), \( h_{i_} \) is the halfwidth of \( P_I \) in the direction of the vector \( u_{i_} \), \( x_I \) is the center point of \( P_I \) and \( D_I \) is the normalizing matrix. Hence, \( P_I + B_l \) is contained in a ball of radius \( R_I \), with
\[
R_I = |D_I^{-1}||W_I^{-1}|h_I + l \leq (3d)^d \sqrt{d} \prod_{i,j \in I, i < j} (i - j)(h + l) < 3^{2d}d^{2d+1/2}(h + l),
\]
where \( h = \max_{1 \leq i \leq 3d} \{h_i\} \) and all matrix norms are those induced by the Euclidean distance. If \( h \leq l \), then each \( P_I \) contains at most one grid point, which contradicts \([13]\) for \( |V| \) large enough, hence \( h > l \), and we have
\[
\text{vol}(P_I + B_l) \leq (h + l)^d \text{vol}(P_I) \leq c_4 h^d.
\]
From this inequality, together with \([14]\) and \([13]\), it follows that
\[
c_5 |V| \leq \left( \frac{h}{l} \right)^d.
\]
This results in the desired lower bound for the width of a slab containing at least \( |V|/3 \) grid points
\[
h \geq c_6 |V|^{1/d}.
\]

Now we show that there is a hyperplane parallel to the boundaries of the slab which intersects at most \( c_6 |V|^{d+1} \) edges of the grid. We divide the slab into \([\frac{1}{2}] \geq c_6 \frac{1}{2} |V|^{1/d} \geq c_7 |V|^{1/d} \) parallel slices of width \( L \). The number of these slices is bigger than 1 if \( |V| \) is sufficiently large. Since the total number of grid points in the slab does not exceed \( |V| \), at least one slice contains fewer than \( c_8 |V|^{d+1} \) grid points.
If a grid edge intersects bisector $H$ of the slice, then at least one end of the edge is inside the slice (since the slice has thickness $L$ and the length of no edge exceeds $L$). Hence, the total number of the edges intersecting $H$ does not exceed $c_8 |V|^{d-1} \delta$, where $\delta$ is the degree of the grid, which is bounded for starry grids. Since $H$ is inside the slab, it separates the grid points into sets containing at least $|V|/3$ points each.

Now we can formulate our covering result, which implies that computations of local operators of fixed order on starry grids can be performed with the same cache efficiency as those on structured grids.

**Theorem 12.** Nodes of $d$-dimensional starry grid $G = (V, E)$ can be covered by sets of size not exceeding $S$ and with total boundary $O(|V| S^{-\frac{d}{2}})$.

**Proof.** The proof closely follows that of the main result of Section 5.1. As was stated in the beginning of the section, any subgrid of a starry grid is starry of the same dimension. Hence, we can construct the covering by applying the Hyperplane Cut Theorem recursively. First, we choose any bisector cutting at most $c_0 |V|^{d-1}$ edges of the grid $G$, where $c_0$ is independent of $G$. According to the Hyperplane Cut Theorem, the bisector can be chosen in such a way that it splits the grid into connected components $G_i = (V_i, E_i)$, $i = 1, \ldots, k$, $|V_i| \leq 2|V|/3$. Adding an extra step in this partition, we can assume that $|V_i| \leq |V|/2$, while the number of edges cut by the bisector does not exceed $c_1 |V|^{d-1}$ for a bigger constant $c_1$. We recursively bisect each connected component $G_i = (V_i, E_i)$ while $|V_i| > S$.

This partition process can be represented by a cut tree $T$ whose nodes are partitioned connected components of the grid. Let a connected component $C$, represented by node $t$ of $T$, be split into components $C_1, \ldots, C_m$ by a hyperplane cut. We draw an edge between $t$ and each of its child nodes representing $C_1, \ldots, C_m$. However, we do not include in $T$ connected components of size smaller than $S$. To each node $t$ of $T$ we assign size $s(t)$, which equals the number of vertices in the set represented by $t$, and weight $w(t) = s(t)^{d-1}$. From the definition of the cut tree it follows that the size of each leaf exceeds $S$. The total number of edges in all cuts can be bounded by $O(\sigma(T))$, where

$$\sigma(T) = \sum_{t \text{ node of } T} w(t)$$

We use two properties of the weights. First,

$$\sum_{t \text{ leaf of } T} w(l) \leq |V| S^{-\frac{d}{2}},$$

since the maximum of $\sum s(l)^{d-1}$ for sizes of the nodes, subject to $\sum s(l) = |V|$ and $s(l) \geq S+1$, is attained at $s(l) = S+1$ for all $l$. Second, as follows from Proposition 14 (see Appendix), for any node $t$ of $T$ we have

$$w(t) < c \sum_{\tau \text{ child of } t} w(\tau)$$
for some $c < 1$ independent of the grid size.

Now $\sigma(T)$ can be estimated in two steps. First, we replace weights in each nonleaf $t$ by the right hand side of (18), going bottom up from the leaves to the root of $T$. This operation will not decrease the total weight. Second, we carry the summation of the new weights across nodes of $T$ by noticing that each leaf $l$ deposits into the total sum $\sigma(T)$ a weight of at most

$$w(l)(1 + c + c^2 + \ldots) = w(l)c_3.$$ 

Hence, it follows from (17) that

$$\sigma(T) \leq c_3|V|S^{-\frac{1}{3}},$$

meaning that the total number of edges in all cuts is $O(|V|S^{-\frac{1}{3}})$. 

### 5.3 Cache Unfriendly three-dimensional Grid

In the previous section we provided a characterization of cache-friendly higher-dimensional unstructured grids, called starry grids. These are not a trivial extension of planar, bounded degree grids to higher dimensions. To demonstrate this, we present a three-dimensional grid of bounded degree that is intrinsically cache-unfriendly. More formally, we construct a three-dimensional grid of $N$ vertices which has a subgrid $G$ of size $cN$ that does not contain small subsets with a small surface-to-volume ratio. Using this property, following the arguments of Section 3, it can be shown that for any computation of a symmetric operator defined on this grid, $\Omega(N/\log S)$ replacement misses must occur.

Our construction is based on embedding an FFT butterfly graph into a triangulation of a three-dimensional cube. The $2^n$-point FFT graph, denoted by $F_n$, has $(n + 1)2^n = N$ vertices, arranged in $n + 1$ layers of $2^n$ vertices each, see Figure 5. In other words, vertices of $F_n$ form an array $(k, i)$, $0 \leq k \leq n, 0 \leq i \leq 2^n - 1$,
and a vertex \((k, i), \ k < n\) is connected with vertices \((k + 1, i)\) and \((k + 1, i \oplus 2^k)\), where \(i \oplus 2^k\) signifies taking the complement of the \(k\)th bit of \(i\).

**Theorem 13.** The number of cache misses \(\mu\) in the evaluation of a symmetric, first-order operator on \(F_n\) is bounded as follows:

\[
\mu \geq \frac{1}{w} N \left(1 + \frac{c}{\log S}\right),
\]

where \(c\) is a constant and \(N = (n + 1)2^n\).

**Proof.** The theorem is a direct sequence of Theorem 3 of Section 3, and of an estimation of the size of the boundary of vertex coverings of \(F_n\), given in Proposition 14. 

**Proposition 14.** Let \(F_n = \bigcup V_i, \ i = 1, \ldots, k\), \(|V_i| \leq S\) be any partition, and \(S \leq 2^{n/24}\). Then the following inequality holds for the sum of the numbers of boundary vertices of the sets of the partition:

\[
\sum_{i=1}^{k} |\partial V_i| \geq \frac{N}{4 \log S}. \tag{20}
\]

**Proof.** For any subset \(V \subset F_n\) it follows from (21) that \(\delta(V) \geq \frac{1}{2}|V|/\log |V|\), and we can estimate the sum of boundaries of the partition as follows:

\[
\sum_{i=1}^{k} |\partial V_i| \geq \sum_{i=1}^{k} \delta(V_i) - 6 \cdot 2^n \geq \frac{1}{2} \sum_{i=1}^{k} \frac{|V_i|}{\log |V_i|} - 6 \cdot 2^n \\
\geq \frac{1}{2 \log S} \sum_{i=1}^{k} |V_i| - 6 \cdot 2^n \geq \frac{N}{4 \log S},
\]

where the boundary operator \(\delta\) is as defined in Lemma 15. The last inequality holds since \(S \leq 2^{n/24}\). 

**Lemma 15.** Let \(V\) be any nonempty node subset of grid \(F_n\), \(n \geq 1\), and let \(E\) be the set of all edges of \(F_n\) incident on at least one node of \(V\). Then we have

\[
|V| \leq 2\delta(V) \log \delta(V), \tag{21}
\]

where \(\delta(V)\) is sum of the number of boundary nodes in \(V\) and of the number of boundary edges of \(E\). A node of \(V\) is called a boundary node if it is in layer 0 or \(n\) of \(F_n\), and an edge of \(E\) is called a boundary edge if it connects a vertex in \(V\) with a vertex not in \(V\).
**Proof.** Our proof of inequality (21) is based on induction and is similar to the proof of Theorem 4.1 in [9]. The base of induction for \( n = 1 \) is obviously true. Next, let \( V \) be partitioned into three sets \( A, B \) and \( C \), as shown in Figure 6. Sets \( A \) and \( B \) contain the nodes of \( V \) that are in the two separate \( F_{n-1} \) subgraphs of \( F_n \). Sets \( A_0 \) and \( B_0 \) are contained in the last layer of these \( F_{n-1} \). Set \( C \) contains the \( n^{th} \) layer of nodes of \( V \) in \( F_n \). The subset of nodes of \( F_n \) that constitutes \( V \) is indicated by open circles.

![Figure 6](image)

**Figure 6.** Induction step for proving the surface-to-volume inequality of a subset in \( F_n \). We can assume without loss of generality that \(|A_0| \geq |B_0|\).

Further, we define the partition \( C = C^2 \cup C^1 \cup C^0 \), where \( C^i \) is the subset of nodes in \( C \) that are adjacent to exactly \( i \) nodes in \( A \cup B \). Now the equality

\[
|V| = |A| + |B| + |C^2| + |C^1| + |C^0|
\]

follows from the fact that \( A \cup B \cup C \) is a partition of \( V \), with \( A \) and \( B \) contained in \( F_{n-1} \).

Now consider those edges of the last layer of \( F_n \) that are incident on a vertex of \( V \). These edges can be partitioned into 5 groups: those incident on nodes in \( A \) and \( C \), \( B \) and \( C \), \( A \) only, \( B \) only, and \( C \) only. We denote these sets by \( E_{AC}, E_{BC}, E_A, E_B \) and \( E_C \), respectively. Since two such edges are incident on each vertex in \( A, B \) and \( C \), we have the following two relations:

\[
|E_A| + |E_{AC}| + |E_B| + |E_{BC}| = 2(|A_0| + |B_0|)
\]

\[
|E_C| + |E_{AC}| + |E_{BC}| = 2|C|
\]

From these equalities it follows that

\[
|E_A| + |E_B| + |E_C| = 2(|A_0| + |B_0| - |C|) + 2|E_C|.
\]

We determine the size of the boundary of \( V \) by adding to \( A \cup B \) the nodes contained in the last graph layer of \( F_n \), i.e. those in \( C \). This causes some boundary
nodes of $A$ and $B$ to cease to be boundary nodes, namely those in $A_0$ and $B_0$, while all nodes in $C$ are now new boundary nodes of $V$. Subsequently, we determine the effect of adding $C$ on the number of boundary edges. It is easy to see that all edges in $V$ that were boundary edges of $A$ or $B$ are also boundary edges of $V$. The boundary edges that are newly created by adding $C$ are those that connect a node of $A_0$ or $B_0$ to a node not in $C$, as well as those that connect a node of $C$ to a node not in $A_0$ or $B_0$. These new edge sets are exactly the following: $E_A$, $E_B$, and $E_C$, which are all disjoint. Consequently, we find:

$$\delta(V) = \delta(A) + \delta(B) - |A_0| - |B_0| + |C| + |E_A| + |E_B| + |E_C|. \quad (22)$$

Taking into account that $|C^2| \leq 2|B_0|$ and that $|E_C| = |C^1| + 2|C^0|$, from the previous equations we derive

$$\delta(V) \geq \delta(A) + \delta(B) + |A_0| - |B_0| + |C^1| + 3|C^0|. \quad (23)$$

Using induction, and assuming that $\delta(B)$ is nonzero, we obtain

$$|V| \leq 2(\delta(A) \log \delta(A) + \delta(B) \log \delta(B) + |B_0|) = 2(\delta(V) \log \delta(V) - X)$$

where

$$X \geq (\delta(A) + \delta(B) + D + |C^1| + 3|C^0|) \log(\delta(A) + \delta(B) + D + |C^1| + 3|C^0|)$$

$$- \delta(A) \log \delta(A) - \delta(B) \log \delta(B) - |B_0|,$$

and $D = |A_0| - |B_0|$. Because $D \geq 0$, $|C^1| + 3|C^0| \geq 0$, and $\delta(A), \delta(B) \geq 1$, we get

$$X \geq \delta(A) \log(1 + \frac{\delta(B)}{\delta(A)}) + \delta(B) \log(1 + \frac{\delta(A)}{\delta(B)}) - |B_0|.$$

Since $|B_0| \leq \delta(B)$ and $|B_0| \leq \delta(A)$ we finally obtain:

$$X \geq |B_0| \log \left[ 1 + \frac{\delta(A)}{\delta(B)} + \frac{\delta(B)}{\delta(A)} \right] / 2 \geq 0. \quad (24)$$

If $\delta(B)$ is zero, the proof simplifies significantly, since now we have to show nonnegativity of $X$, with

$$X \geq (\delta(A) + |A_0| + |C^1| + 3|C^0|) \log(\delta(A) + |A_0| + |C^1| + 3|C^0|) - \delta(A) \log \delta(A), \quad (25)$$

which is trivial, since $\delta(A) \geq 1$. \[Q.E.D.\]

The FFT graph can be embedded into a triangulation of a three-dimensional cube. An inductive step of embedding of the FFT graph into a triangulation of simplices is shown in Figure 7. The simplices can be embedded into a cube, as shown in Figure 3, which then can be partitioned into parallelepipeds. Finally, each such parallelepiped can be triangulated.
Assuming that we have an embedding of the edges connecting the last two layers of $F_{n-1}$ (butterflies) into the triangulation of a simplex, we embed the butterflies connecting the last two layers of $F_n$ into a triangulation of a simplex. We map the vertices of the last two layers $F_n$ into equidistant points on two crossing edges of a simplex, see Figure 7. If we linearly parametrize these crossing edges and connect corresponding points by lines, we build a ruled surface. A ruled surface can be viewed as a hyperboloid containing the two crossing edges and the connecting lines. Each ruled surface separates a simplex built on the appropriate vertices into two parts, as shown in Figure 10; the top view is shown in Figure 9.

We map the edges of the butterflies onto lines of one of the ruled surfaces separating simplices $(t_0, t_3, b_7, b_4)$ and $(t_7, t_4, b_3, b_0)$ and two other ruled surfaces separating simplices $(t_0, t_3, b_3, b_0)$ and $(t_7, t_4, b_4, b_7)$, respectively. The whole simplex $(t_0, t_7, b_7, b_0)$ can be partitioned into the four simplices listed above, and 5 primitive simplices which will not be further partitioned: $(t_3, t_4, b_3, b_4), (t_3, t_4, b_4, b_7), (t_3, t_4, b_3, b_0), (t_0, t_3, b_4, b_3)$ and $(t_7, t_4, b_4, b_3)$. Each of the simplices $(t_0, t_3, b_7, b_4), (t_7, t_4, b_3, b_0), (t_0, t_3, b_3, b_0)$ and $(t_7, t_4, b_3, b_0)$ is divided by a ruled surface, hence it is sufficient to build a triangulation of a simplex separated by a ruled surface. This can be done in 2 steps: 1. partitioning the simplex into prisms by planes parallel to the other crossing edges of the simplex (see Figure 10), and 2. triangulating each of the prisms into primitive simplices.

Finally, we embed the triangulated simplices into a cube and augment it by a triangulation of the space between simplices and the cube, as shown in Figure 8.

It is easy to verify that the total number of vertices in the triangulation does not exceed $M = 3n2^n$, and that the degree of each node does not exceed 16. Hence we have constructed a triangulation having the property declared at the beginning of this section.

![Figure 7. Recursive construction of embedding of FFT graph into a triangulations of a simplex.](image)

![Figure 8. (Partial) recursive triangulation of a cube (view rotated with respect to Fig. 7).](image)
6 Related Work and Conclusions

Because of the growing depth of memory hierarchies and the concomitant increase in data access times, the reduction of cache misses in scientific computations remains an active subject of research. One of the first lower bounds for data movement between primary and secondary storage was obtained in [9]. Recent work has focused on developing compiler techniques to reduce the number of cache misses. In this direction we mention [7], where the notion of cache miss equation (CME) and a tiling of structured grids with conflict-free rectilinear parallelepipeds were introduced. Some tight lower and upper bounds for computation of local operators of fixed radius on structured grids were obtained in [8], where a tiling with a reduced fundamental parallelepiped of the interference lattice was used for reduction of cache misses. Some practical methods for improving cache performance in computations of local operators are given in [10].

In this paper we showed that the reduction of cache misses for computations of local operators of fixed radius, defined on structured or unstructured discretization grids, is closely related to the problem of covering these grids with conflict-free sets having low surface-to-volume ratio. We introduced two new coverings of structured grids: one with Voronoi cells, and one with rectilinear parallelepipeds built on the vectors of successive minima of the grid interference lattice. The cells of both coverings have near-minimal surface-to-volume ratios. Direct measurements of cache misses show a significant advantage of the successive minima covering relative to computations using the natural loop order, maximally optimized by a compiler. We also showed that the computation of local operators of fixed radius on planar unstructured grids can be organized in such a way that the number of cache misses is asymptotically close to that on structured grids. Finally, we demonstrated how
the latter result can be extended to higher dimensions.

**Appendix: The Weight Inequality**

**Proposition 16.** For any positive \( v_1 \geq \cdots \geq v_k > 0 \) such that \( v_1 \leq \sum_{i=2}^{k} v_i \), the following inequality holds:

\[
\sum_{i=1}^{k} v_i^{1/d} \geq \left( \frac{2}{\sum_{i=1}^{k} v_i} \right)^{1/d}.
\]

**Proof.** The proof uses Jensen inequality, see [5], Ch 2.10, Th. 19: for \( 0 < r < s \)

\[
(\sum_{i=1}^{k} v_i^{1/r})^r \leq (\sum_{i=1}^{k} v_i^{1/s})^s
\]

and in particular

\[
(\sum_{i=1}^{k} v_i^d)^{1/d} \leq \sum_{i=1}^{k} v_i \leq (\sum_{i=1}^{k} v_i^{1/d})^d
\]

Let \( x_i = v_i^{1/d}, \; i = 1, \ldots, k \), we have to prove

\[
(\sum_{i=1}^{k} x_i)^d \geq 2 \sum_{i=1}^{k} x_i^d
\]

where \( x_1 \leq (\sum_{i=2}^{k} x_i^d)^{1/d} \leq \sum_{i=2}^{k} x_i \) and \( x_1 \geq \cdots \geq x_k > 0 \).

Let \( j < k \) be the minimal index such that \( x_j > \sum_{i=j+1}^{k} x_i \). Obviously, \( j > 1 \), so we have:

\[
(\sum_{i=1}^{k} x_i)^d \geq \sum_{i=1}^{k} x_i^d + d x_1^{d-1} \sum_{i=2}^{k} x_i + \cdots + d x_{j-1}^{d-1} \sum_{i=j}^{k} x_i + \sum_{i=j+1}^{k} x_i
\]

\[
> \sum_{i=1}^{k} x_i^d + d x_1^d + \cdots + d x_{j-1}^d (x_{j+1} + \cdots + x_k)
\]

\[
\geq \sum_{i=1}^{k} x_i^d + d x_1^d + \cdots + d x_{j-1}^d + d x_{j+1}^d + \cdots + d x_k^d > 2 \sum_{i=1}^{k} x_i^d
\]

since \( d \geq 2 \). If no such \( j \) exists then the proof becomes even simpler.
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