Analysis of Layered Hierarchy for Necklaces

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1 Introduction

Molecular configurations can be modeled as sets of spheres in 3D. By imposing geometric constraints on the spheres based on molecular biology one can apply efficient techniques [3], for example, to analyze the complexity of molecular surface [1]. Guibas *et al.* [2] introduced a model called *necklace* that finds applications in computer graphics, computer vision, robotics, geographic information systems and molecular biology. They studied two data structures, *wrapped hierarchy* and *layered hierarchy*, for representing necklaces and for performing collision tests.

Guibas *et al.* [2] proved that the wrapped hierarchy admits a separating family of size $O(n^{2-2/d})$. This is the first subquadratic bound proved for collision detection using predefined hierarchies. Although the layered hierarchy can be used for collision detection, "no subquadratic bound on the size of a separating family based on the layered hierarchy is currently known" [2]. The main result of this paper is that the same upper bound holds for the layered hierarchy.

One of the advantages of layered hierarchy over wrapped hierarchy is the "local" definition of the cages. We propose a modification of the layered hierarchy so that some deformations of a necklace can be maintained efficiently. In particular, we show that *rigid-body conformational changes* can be handled in $O(\log n)$ time only.

2 Necklaces and Bounding-Volume Hierarchies

We define the notion of necklace in a slightly more general form[1].

Definition 1 (Necklace) *A* necklace *is a sequence of beads $\mathcal{N}=\langle B_1, B_2, \ldots, B_n\rangle$ in $\mathbb{R}^d$ space that has the following properties:*

1. *The radius of each bead is in the interval $[\rho_{\min}, \rho_{\max}]$ where $\rho_{\min}, \rho_{\max}$ are positive constants.*
2. *The distance between the centers of two adjacent beads is bounded by a constant δ.*

Collision detection problem arises in such applications as protein folding and protein docking. A bounding volume hierarchy is a common approach that models and detects collisions and self-collisions of different geometrical shapes including necklaces. This approach reduces computational time since it suffices to test collisions among bounding volumes.

Definition 2 (Hierarchies) *For a necklace $\mathcal{N}$, let $T(\mathcal{N})$ denote the balanced binary tree defined recursively so that, for an internal node v, its left subtree contains $\lfloor m/2 \rfloor$ leaves where m is the number of leaves below v. Both wrapped and layered hierarchies have a* cage *$C(v)$ associated with a node v of $T(\mathcal{N})$ and the cages of leaves correspond to the beads, $C(v) = B_i$ for i-th leaf v where $i = 1, 2, \ldots, n$. For an internal node v, the cage is defined differently for two hierarchies:*

- Wrapped hierarchy. *The cage $C(v)$ is the smallest enclosing ball of beads corresponding to the leaves below v.*
- Layered hierarchy. *The cage $C(v)$ is the smallest enclosing ball of the cages corresponding to the children of v.*

The layered hierarchy has many advantages over the wrapped counterpart. For a necklace size n, the layered hierarchy can be constructed in linear time since the cage of each node can be computed in $O(1)$ time. The wrapped hierarchy can be constructed in $O(n \log n)$ time by using linear-time algorithm [4] for computing the minimum enclosing sphere MES. A simpler algorithm for computing MES in expected $O(n)$ time can be used. Note that the algorithm for the layered hierarchy is even simpler.

3 Necklace Deformation with Layered Hierarchy

Modeling conformation changes is required in protein docking, robotics and computer graphics. One

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[1] We do not require that any two consecutive beads along the necklace have a point in common.

type of local deformation - *rigid-body conformational change* [5] - can be defined as follows.

Definition 3 (Conformational Change) *Let $\mathcal{N} = \langle B_1, B_2, \ldots, B_n \rangle$ be a necklace and let i be an index from 1 to $n-1$. Let M be a rigid motion in $\mathbb{R}^3$ (the composition of a translation and a rotation). If $\mathcal{N}' = \langle B_1, \ldots, B_i, M(B_{i+1}), \ldots, M(B_n) \rangle$ is a necklace then $\mathcal{N}'$ is a rigid-body conformational change of $\mathcal{N}$.*

We show how to modify the layered hierarchy so that a rigid-body conformational change can be done efficiently. We store a rigid motion $M(v)$ associated with a vertex v of $T(\mathcal{N})$. Each rigid motion $M(v)$ is a composition of a 3D rotation $R(v)$ and a translation $T(v)$. The rotation can be represented as a quaternion or a rotation matrix. We assume that the inverse rigid motion $M^{-1}(v)$ can be computed in $O(1)$ time. We call the hierarchy augmented with rigid motions as *augmented layered hierarchy*.

The augmented layered hierarchy defines the position of a bead B_i in the space as follows. Let $v_1 = v_{\text{root}}, v_2, \ldots, v_k$ be the path from the root of the layered hierarchy to the vertex with the bead B_i and let c_i be the center of the bead stored in v_k. Then the real position of B_i is $M_1(M_2(\ldots M_k(c_i)\ldots))$ where $M_j = M(v_j), j = 1, \ldots, k$. Let I denote the *identity transformation*, i.e. $I(p) = p$ for any $p \in \mathbb{R}^3$.

Theorem 1 *The augmented layered hierarchy can be maintained in $O(\log n)$ time if a rigid-body conformational change is applied.*

4 Cages of Layered Hierarchy

Although the layered hierarchy can support rigid-body conformational changes efficiently (if augmented as in previous section), the wrapped hierarchy occupies smaller space since its cages are always no larger that the corresponding cages of the layered hierarchy. Despite this evidence we show that the cages of the layered hierarchy have the same upper bound as the corresponding cages of the wrapped hierarchy.

Let T_u denote the subtree rooted at a vertex u of $T(\mathcal{N})$ and let $n_l(u)$ be the number of leaves in T_u.

Theorem 2 *The radius of any cage $C(v)$ of layered hierarchy $T(\mathcal{N})$ is at most $\delta(n_l(v)-1)/2 + \rho_{\max}$, where $n_l(v)$ is the number of leaves for a tree is rooted at v.*

5 Collision Detection for Layered Hierarchy

An useful tool for the collision testing is a *separating family* [2].

Definition 4 (Separating Family) *A* separating family $\Sigma = \{(u, v)\}$ *is a set of pairs of nodes of a volume bounding hierarchy satisfying the following properties:*

1. *If $(u, v) \in \Sigma$ then $C(u)$ and $C(v)$ are disjointed.*
2. *For any two non-adjacent beads $B_p, B_m \in N$, there is a pair $(u, v) \in \Sigma$ such that $B_p \subseteq C(u)$ and $B_m \subseteq C(v)$.*

To derive a bound for the layered hierarchy we analyze a separating family Σ built by the following algorithm for collision detection. The algorithm starts with the pair $Q = \{(root, root)\}$ and, for a pair $(u, v) \in Q$ such that $C(u) \cap C(v) \neq \emptyset$, replaced it by at most 4 pairs of children of u and v. Our analysis is based on the analysis of the wrapped hierarchy by Guibas *et al.* [2].

Lemma 3 *If $(C(u), C(v)) \in \Sigma$ then the cage $C(v)$ is contained in $K - C(u)$ where K is the ball concentric with $C(u)$ and of radius $4(\delta n_l(u) + \rho_{\max})$.*

Theorem 4 *Let $\mathcal{H}_L$ be the layered hierarchy for a necklace $\mathcal{N}$ in $\mathbb{R}^d, d \geq 3$ with n beads. Algorithm 2 builds the unique separating family Σ for $\mathcal{N}$ of size $O(n^{2-2/d})$. This bound is asymptotically tight in the worst case.*

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