



Analytic methods for geometric modeling via spherical decomposition[☆]



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HIGHLIGHTS

- We propose a grid-free discretization scheme for analytic geometric modeling.
- Solids are approximated with countable unions of 3D balls cut from 4D cones.
- The unions turn into 3D slices of 4D Minkowski sums of knots and a template cone.
- The Minkowski formulation embeds well into cross-correlations between solids.
- The analytic formulation follows using convolution algebra and Fourier Transform.

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ABSTRACT

Analytic methods are emerging in solid and configuration modeling, while providing new insights into a variety of shape and motion related problems by exploiting tools from group morphology, convolution algebras, and harmonic analysis. However, most convolution-based methods have used uniform grid-based sampling to take advantage of the fast Fourier transform (FFT) algorithm. We propose a new paradigm for more efficient computation of analytic correlations that relies on a grid-free discretization of arbitrary shapes as countable unions of balls, in turn described as sublevel sets of summations of smooth radial kernels at adaptively sampled 'knots'. Using a simple geometric lifting trick, we interpret this combination as a convolution of an impulsive skeletal density and primitive kernels with conical support, which faithfully embeds into the convolution formulation of interactions across different objects. Our approach enables fusion of search-efficient combinatorial data structures prevalent in time-critical collision and proximity queries with analytic methods popular in path planning and protein docking, and outperforms uniform grid-based FFT methods by leveraging nonequispaced FFTs. We provide example applications in formulating holonomic collision constraints, shape complementarity metrics, and morphological operations, unified within a single analytic framework.

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1. Introduction

Analytic modeling relies on describing shape and configuration pointsets as sublevel sets of functions and formulating fundamental operations (e.g., pertaining to detecting collisions, similarity, complementarity, or symmetry) in terms of correlations between those functions. For example, Minkowski operations [1] that are central to mathematical morphology are formalized as convolutions of constituent functions and computed efficiently

in the Fourier domain [2]. Minkowski operations have been used extensively to formulate important problems in robot path planning [3], mechanism workspace design [4], virtual reality (graphics/haptics) [5,6], protein docking [7], packaging and nesting [8], and more. Unfortunately, their combinatorial computation even for 3D polyhedral objects quickly becomes impractical with increasing number of polygons [2]. This can be alleviated using classical FFTs [9] for numerical implementation of convolutions, which take advantage of uniform spatial sampling. However, this and several related correlation-based problems can be solved more efficiently by using a spherical decomposition of the shape and nonuniform FFTs [10]. Here we briefly review the roots of the main ideas, with a focus on collision detection (CD) and shape complementarity (SC) literature.

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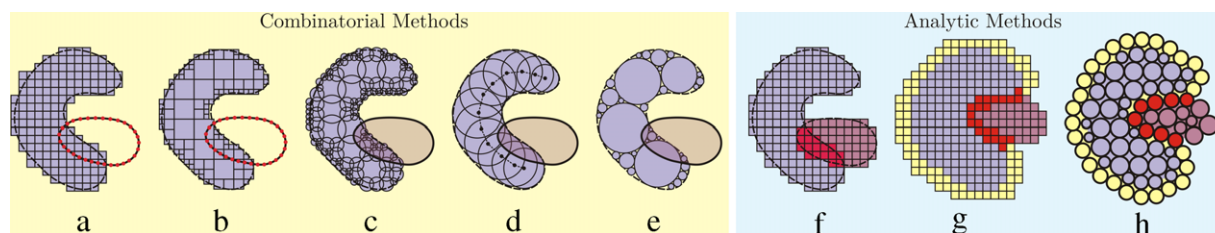


Fig. 1. Research in combinatorial methods has shown that CD tests over uniform grids (i.e., ‘voxmaps’) [11] (a) and octrees (special case of OBB-trees) [12] (b) can be made more efficient if voxels are replaced with spherical primitives, e.g., built around octrees [13] (c), sampled over the MA [14,15] (d) or packed inside using distance fields [16] (e). However, the more nascent analytic methods are still mostly reliant on uniform grids for, e.g., CD testing for solids by integrating the intersection [17] (f), and SC scoring for proteins by integrating skin overlaps [18] (g). The latter has been outperformed by grid-free correlations of atoms grouped with equal radii [7] (h). We show that constructions in (c)–(e) with arbitrary radii can also be interpreted analytically as a convolution and solved by nonuniform FFTs after a geometric lifting.

1.1. Background

At one end of the research spectrum are combinatorial techniques that use surface meshes or higher-order algebraic parametrizations to resolve collisions or identify matching features. Examples are polyhedral CD methods based on Voronoi-clipping/marching [19] and oriented bounding box (OBB) trees [12], or spatial enumeration-based techniques such as the Voxmap PointShell (VPS) [11]. VPS works by a pairwise test between a shell of vertices for the moving object against a map of voxels that discretizes the stationary obstacle, and is popular in physically-based modeling in virtual environments [20]. Others have identified more efficient techniques for time-critical CD by using hierarchical bounding spheres sampled on octrees [13] or on the medial axes (MA) [14,15], and interior sphere packing guided by distance fields [16] (Fig. 1(a)–(e)). These ‘sphere-tree’ based methods have been shown to outperform voxmap or OBB-tree based techniques in real-time applications [16] – particularly because primitive collision predicates are simplified to center-distance tests as a result of the orientational symmetry of balls – and are considered state-of-the-art in practice. For a more complete survey on CD methods, we refer the reader to [21].

On the other end of the spectrum are analytic methods that have been more popular in robotics [3]. Unlike the combinatorial approach that searches for a collision certificate point (or lack thereof) in the intersection of the objects, the analytic approach treats the collision predicate as a Boolean combination of inequalities over some configuration space of the objects [22]. The obstacle avoidance in path planning is, for example, treated as an optimization problem subjected to holonomic collision constraints formulated analytically as a convolution of the robot and its workspace [17]. Most convolution-based methods have so far focused on generating uniformly sampled configuration bitmaps for all spatial positions and orientations simultaneously, which can be cumulatively computed with asymptotically optimal FFTs [9]. However, a complete description of the configuration obstacle is overkill for real-time CD. A recent work [22], also reliant on uniform grid-based sampling, formally reframes the approach for time-critical CD (Fig. 1(f)), but has not yet been compared with sphere-tree methods, nor applied to real-time applications.

In an independent line of research, numerous analytic methods for molecular surface analysis and SC-based protein docking have been developed, whose outcomes are platforms that use grid-based occupancy enumeration and leverage classical FFTs [9] such as ZDock [18], or more recent grid-free techniques that rely on nonuniform FFTs [10], such as F²Dock [7] (Fig. 1(g), (h)). The latter exploits the spherical shape of the atomic building blocks and implicitly represents the proteins as summations of radial kernels centered around atoms, assigning different weights to core and skin atoms. The SC score is obtained by cross-correlating these functions from different proteins, which turns into a convolution discretized over the center points. It has been shown that grid-free

methods outperform uniform grid-based methods [7] by taking advantage of the spherical geometry. A comprehensive survey on advances in protein docking is available in [23].

Although objects of arbitrary shape, unlike molecules, cannot be represented *exactly* as finite unions of balls, the sphere-tree methods for time-critical CD were shown to be more successful in progressively approximating the shape, when compared to uniform grid- or octree-based voxelization, with a faster convergence and a better use of computational resources [14]. Motivated by this observation, we present a generic framework for representing arbitrary shapes with finite (or countably infinite, in the limit) radial kernels, formulated as a convolution of a discrete pointset and the primitive kernel in a higher-dimensional space. The latter is described as a *geometric lifting* trick in Section 2.2, and is deemed necessary due to the inevitable size difference between primitive balls, unlike the simpler case for the proteins. We show that this approach offers ‘the best of both worlds’ by combining the computational efficiency of the sphere-tree techniques for time-critical applications (i.e., with a single configuration query) with that of the analytic methods for cumulative configuration space constructions (i.e., requiring a complete map for all spatial relations), unified under a single paradigm with analytic formalism that applies to a multitude of applications.

1.2. Contributions

The main contributions of this paper are to (1) present an analytic shape correlation paradigm centered around a nonuniform discretization scheme¹ that relies on progressive spherical approximations with balls of different sizes; and (2) a uniform and efficient approach to solving a variety of problems that deal with detecting collisions, shape similarity/complementarity, and shape morphing, examples of which we describe in Section 4.

Moreover, we show that the spherical discretization offers an algebraic structure that is closed under Minkowski sum/product operations, and at the same time offers more appealing properties than uniform grid- or octree-based discretizations. As the continuous geometry (of both shapes and configurations) is abstracted away by the balls, the computational implementation solely relies on convolution algebra over discrete sets specified completely by ball center coordinates and radii, allowing the use of the efficient nonequispaced FFT (NFFT) algorithm [10] on the highly parallel graphics processing units (GPU) [24].

¹ What we mean by a ‘discretization scheme’ is not a particular decomposition algorithm or approximation method, but a generic formalism for reconciling such a nonuniform discretization (in contrast to the extensively used uniform sampling) to analytic modeling, using Minkowski sums and convolutions. We do present one new algorithm in Appendix A; nevertheless, other methods [13–16] are also applicable under the same scheme.

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