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Equidistributed icosahedral configurations on the sphere

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ABSTRACT

We present and analyze a new sequence of equidistributed icosahedral configurations. These configurations are created by combining the (m, n) icosahedral nodes of Caspar and Klug and adapting the azimuthal projection method of Snyder to create a low deformation equal area mapping from the regular icosahedron to $\mathbb{S}^2$. We prove an upper bound on the mesh ratio of these configurations and analyze numerically the Riesz potential energies of the point sets of size $N < 50{,}000$.

1. Introduction and main results

Point generation on the sphere is widely studied in math subfields such as numerical analysis, approximation theory, and PDE's as well as in a breadth of disciplines within physics, biology, chemistry, and the geosciences. Many spherical point sets have been developed for a variety of specific models (see for example [1–7]), and each configuration has various desirable properties [8]. Caspar and Klug [9] in their study of spherical viruses and particle protein arrangements created a now well known icosahedral point configuration which we describe below. Radial projection of the Caspar–Klug (CK) nodes results in a sequence of spherical configurations.

The purpose of this paper is to improve upon these configurations by implementing an area preserving map Φ from the regular icosahedron $\mathcal{I}$ of surface area 4π to the unit sphere $\mathbb{S}^2$ with low angular deformation and study the image of the CK configurations under Φ. We create this map by adapting the azimuthal equal area method presented by Synder for the truncated icosahedron [10]. These new configurations are equidistributed and have advantages in mesh ratio and Riesz potential energy over a wide variety of popular configurations on the sphere including the radially projected CK configurations.

The CK configurations on $\mathcal{I}$ are constructed as follows: Consider the planar triangular lattice generated by $\vec{e}_1 = (1, 0)$ and $\vec{e}_2 = (1/2, \sqrt{3}/2)$. For a given $(m, n) \in \mathbb{N}^2 \setminus (0, 0)$, let $\vec{e}_{m,n} = m\vec{e}_1 + n\vec{e}_2$ and its rotation by $\pi/3$ be basis vectors for an unfolded icosahedron superimposed on the lattice as illustrated in Fig. 1. Folding the icosahedron results in a triangular lattice on each face. Due to rotational symmetry of the lattice, the resulting configuration is independent of the planar unfolding of the icosahedron. The total number of points in an (m, n) configuration is

$$N = 10(m^2 + mn + n^2) + 2$$

which can be seen by examining a half open fundamental domain generated by $\vec{e}_{m,n}$ and its rotation by $\pi/3$. The CK structures have been physically realized in viral capsids (cf. [11,12]). As point sets they have been well studied as candidates for low energy configurations and are known to be local minima for the Coulomb energy when projected radially to the sphere [13–15,8].

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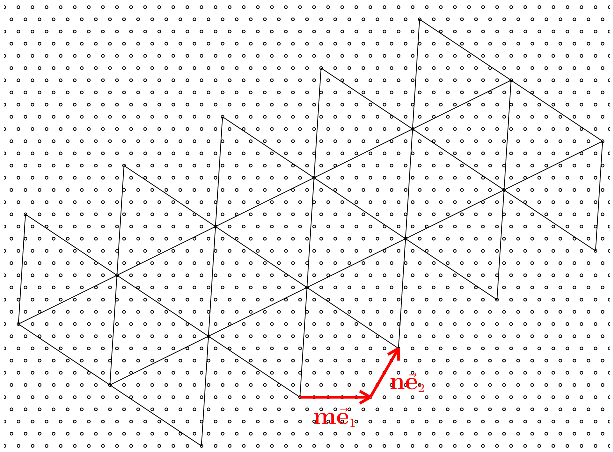

Fig. 1. Planar icosahedral mesh for $(m, n) = (5, 4)$.

The sequence of spherical CK configurations noticeably lacks *equidistribution*, a property necessary in low error numerical integration [16,17], digitizing $\mathbb{S}^2$ for computer graphics purposes [18], as well as in minimizing a class of discrete potentials [19]. For a compact surface A, let σ_A be the normalized surface area measure on A. A sequence $\{\omega_N\}_{N=1}^{\infty}$ of point sets in A is called *equidistributed* if for all convex sets $B \subset A$ with $\sigma_A(\partial B) = 0$

$$\lim_{N\to\infty} \frac{\#B \cap \omega_N}{\#\omega_N} = \sigma_A(B) \tag{1}$$

where # denotes cardinality. Indeed, the CK configurations are equidistributed on the icosahedron, but radial projection is not area preserving. By projecting the CK nodes by the equal area mapping Φ described in Section 2, the resulting sequence of configurations will be equidistributed on $\mathbb{S}^2$.

Several alternative methods for generating a sequence of equidistributed icosahedral spherical point configurations have been put forth [20–23]. Some of these approaches are non deterministic and they generate points along the subsequence $(m, 0)$. One advantage of the CK configurations is that they are defined for many values of total points N. The following number theoretic result is interesting from this perspective.

Proposition 1. *Let* $T := \left\{x = 10(m^2 + mn + n^2) + 2 \mid m, n \in \mathbb{N}\right\}$ *and let*

$$S(N) := |\{x \in T \mid x \le N\}|.$$

Then,

$$S(N) = O\left(\frac{N}{\sqrt{\log N}}\right). \tag{2}$$

By comparison, for points generated along the subsequence $(m, 0)$, the analogous quantity $S(N) = O(\sqrt{N})$. A proof of Proposition 1 is given in Section 4.

For the study of local statistics, separation and covering properties play an important role. The *separation* of an N-point configuration ω_N is

$$\delta(\omega_N) := \min_{\substack{x,y\in\omega_N \\ x\neq y}} |x - y|,$$

and the *covering radius* of ω_N with respect to $\mathbb{S}^2$ is defined to be

$$\eta(\omega_N) := \max_{y\in\mathbb{S}^2} \min_{x\in\omega_N} |x - y|.$$

A sequence of N-point configurations $\{\omega_N\}_{N=2}^{\infty}$ is said to be *quasi-uniform* if the sequence

$$\gamma(\omega_N) := \frac{\eta(\omega_N)}{\delta(\omega_N)}, \quad N \ge 2,$$

is bounded as $N \to \infty$. The quantity $\gamma(\omega_N)$ is called the *mesh ratio* of ω_N. Note that some authors define the mesh ratio as $2\gamma(\omega_N)$. We remark that equidistribution does not imply quasi-uniformity or vice versa. In applications involving radial basis

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