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UNIFORMITY DEGREE OF SOME SPHERICAL GRIDS USED IN MAGNETIC RESONANCE POWDER SIMULATIONS

C. CRĂCIUN[1*]

ABSTRACT. This paper compares the uniformity degree of nine spherical grids used in magnetic resonance powder simulations. The comparison is based on known mesh quality measures, which depend on the grid points and the generated Voronoi regions on the unit sphere. According to computations, the distributions of the grids' geometric properties characterise better the grids' quality then the global uniformity metrics.

Keywords: *spherical grid, uniformity degree, Voronoi cell*

INTRODUCTION

The spherical grids used in magnetic resonance powder simulations have been previously assessed using three approaches. The first approach computes geometric homogeneity metrics, depending on the grid points' location on the unit sphere and the generated Voronoi tessellation [1]. The second approach compares the grids based on the quality of their magnetic resonance simulations [2,3]. The third approach, used in the context of continuous-wave electron paramagnetic resonance (CW EPR) powder simulations, is based on EPR-related metrics [4]. These EPR metrics depend on the distribution of the resonance magnetic fields inside the grids' Voronoi regions.

This paper follows the first approach and computes other uniformity metrics than previously reported for nine spherical grids. The metrics are known mesh quality measures and have been selected from those presented in references [5,6].

The paper is structured as follows. The *Theoretical details* section presents the uniformity metrics. The *Computational details* section describes the numerical methods and the software used in calculations. The results and the grids' comparison are given in the *Results and discussion* section. Final section summarizes current work.

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[1] *Babeş-Bolyai University, Faculty of Physics, 1 Kogălniceanu str., 400084 Cluj-Napoca, Romania.*
* *Corresponding author e-mail: cora.craciun@phys.ubbcluj.ro*

THEORETICAL DETAILS

For each grid, let P_k, for k = 1,...,N, be the grid points located on the unit sphere. Each grid point P_k is characterised by its Cartesian coordinates, given as a column vector $\boldsymbol{x_k}$. Let denote by V_k the Voronoi cell generated by P_k on the unit sphere. The uniformity metrics computed in this paper are the following [5,6]:

1. The mesh rati

$$\gamma = \frac{\max_{k=1,\dots,N} \gamma_k}{\min_{k=1,\dots,N} \gamma_k} - 1,$$

where γ_k is the minimum Euclidean distance between the grid point $\boldsymbol{x_k}$ and the other grid points [5]:

$$\gamma_k = \min_{j=1,\dots,N, j\neq k} \left| \boldsymbol{x_k} - \boldsymbol{x_j} \right|, \text{ for k = 1,...,N.}$$

2. The covariance measure

$$\lambda = \frac{1}{\bar{\gamma}} \left[\frac{1}{N} \sum_{k=1}^{N} (\gamma_k - \bar{\gamma})^2 \right]^{1/2} = \left[N \frac{\sum_{k=1}^{N} \gamma_k^2}{\left(\sum_{k=1}^{N} \gamma_k \right)^2} - 1 \right]^{1/2},$$

where $\bar{\gamma} = \frac{1}{N} \sum_{k=1}^{N} \gamma_k$. The covariance measure represents the relative standard deviation of the γ_k values.

3. The regularity measure

$$\chi = \max_{k=1,\dots,N} \chi_k - 1,$$

where

$$\chi_k = \sqrt{3} h_k / \gamma_k \text{ , for k = 1,...,N,}$$

and h_k is the maximum Euclidean distance between the grid point $\boldsymbol{x_k}$ and the other points of the Voronoi cell V_k:

$$h_k = \max_{y \in V_k} \left| \boldsymbol{x_k} - \boldsymbol{y} \right|, \text{ for k = 1,...,N.}$$

As in reference [4], each h_k value may be approximated with the Euclidean distance between the grid point $\boldsymbol{x_k}$ and the furthermost vertex of its Voronoi cell.

4. The second moment trace measure

$$\tau = \max_{k=1,\ldots,N} \left| T_k - \overline{T} \right|$$

where:

$$T_k = \mathrm{trace}(\boldsymbol{M_k}), \text{ for k = 1,...,N, and } \overline{T} = \frac{1}{N}\sum_{k=1}^{N} T_k .$$

$\boldsymbol{M_k}$ is the second moment tensor of the Voronoi cell V_k [6]:

$$\boldsymbol{M_k} = \frac{1}{M_k}\int_{V_k} (\boldsymbol{x} - \overline{\boldsymbol{x}}_{\boldsymbol{k}})(\boldsymbol{x} - \overline{\boldsymbol{x}}_{\boldsymbol{k}})^T \; d\boldsymbol{x}$$

where M_k is the zeroth moment (the mass) of V_k:

$$M_k = \int_{V_k} d\boldsymbol{x}$$

and $\overline{\boldsymbol{x}}_{\boldsymbol{k}}$ is the first moment (the centre of mass) of V_k:

$$\overline{\boldsymbol{x}}_{\boldsymbol{k}} = \frac{1}{M_k}\int_{V_k} \boldsymbol{x} \; d\boldsymbol{x} .$$

The integral in the expression of the second moment tensor $\boldsymbol{M_k}$ may be computed probabilistically, by randomly sampling the Voronoi cell V_k with N_k points, $\boldsymbol{y_j}$, for j = 1,...,N_k [6]:

$$\boldsymbol{M_k} = \frac{1}{N_k}\boldsymbol{S_k} - \overline{\boldsymbol{x}}_{\boldsymbol{k}}\overline{\boldsymbol{x}}_{\boldsymbol{k}}^{\,T}$$

where:

$$\overline{\boldsymbol{x}}_{\boldsymbol{k}} = \frac{1}{N_k}\sum_{\boldsymbol{y}_j \in V_k} \boldsymbol{y}_j \text{ and } \boldsymbol{S_k} = \sum_{\boldsymbol{y}_j \in V_k} \boldsymbol{y}_j \boldsymbol{y}_j^{\boldsymbol{T}} .$$

Smaller values of all these uniformity metrics correspond to more uniform grids [5].

COMPUTATIONAL DETAILS

The spherical grids compared in this paper (with abbreviation and size given in parenthesis) are the following: Igloo (562) [7], Lebedev (Leb, 590) [8-13], Spiral (578) [14], Fibonacci (Fib, 579) [15], the Zaremba, Conroy, and Wolfsberg grid (ZCW, 610) [16-18], the golden ratio-based ZCW (ZCW-n, 578) [4], the Alderman-Solum-Grant grid (ASG, 578) [19], SOPHE (578) [20], and EasySpin (ES, 578) [1,21]. More details about these grids, their generation and random sampling may be found in references [1,2,4]. The Voronoi tessellation of the grids was computed using the STRIPACK package (R.J. Renka) [22], in the implementation available at [23] (stripack.f90, version 2007). For the second moment trace measure, the grids' Voronoi cells were randomly sampled using the J. Arvo's stratified sampling procedure for spherical triangles [24,25] and the pseudo-random number generator from GNU Octave [26,27]. The random sampling was repeated three times for each grid. The spherical grids were sampled with about 392000 random points, as described in [4]. The figures were generated within the R software environment [28].

RESULTS AND DISCUSSION

1. Distribution of the grids' geometric properties

The uniformity metrics presented in this paper depend on geometric quantities calculated for all grid points or for all Voronoi cells of a spherical grid. The mesh ratio γ and the covariance measure λ depend on the shortest distances γ_k (k = 1,...,N) between the grid points. The regularity measure χ depends on the χ_k values, which are directly proportional to the longest distances h_k between the grid points and the other points of the corresponding Voronoi cells, and inversely proportional to γ_k. The τ measure depends on the traces T_k of the second moment tensors of the Voronoi cells.

Figure 1 shows the distributions of the γ_k, χ_k, and T_k values for the nine investigated grids, in beanplot and boxplot representation [28]. In case of T_k, one out of three distributions obtained by each grid's random sampling is presented. The median, range, and interquartile range (IQR) [28] of the distributions are given in Table 1. The grids have close median values for the same type of distribution and therefore we focus on the range and IQR values.

a) The Spiral, Igloo, ZCW, ZCW-n, and Fibonacci grids have less distributed γ_k values (lower IQR) than the other grids. This shows that, for these grids, the shortest distances between the grid points are highly homogeneous on the whole unit sphere. The γ_k distributions for Spiral, ZCW, and ZCW-n, however, have high range due to some extreme outliers.

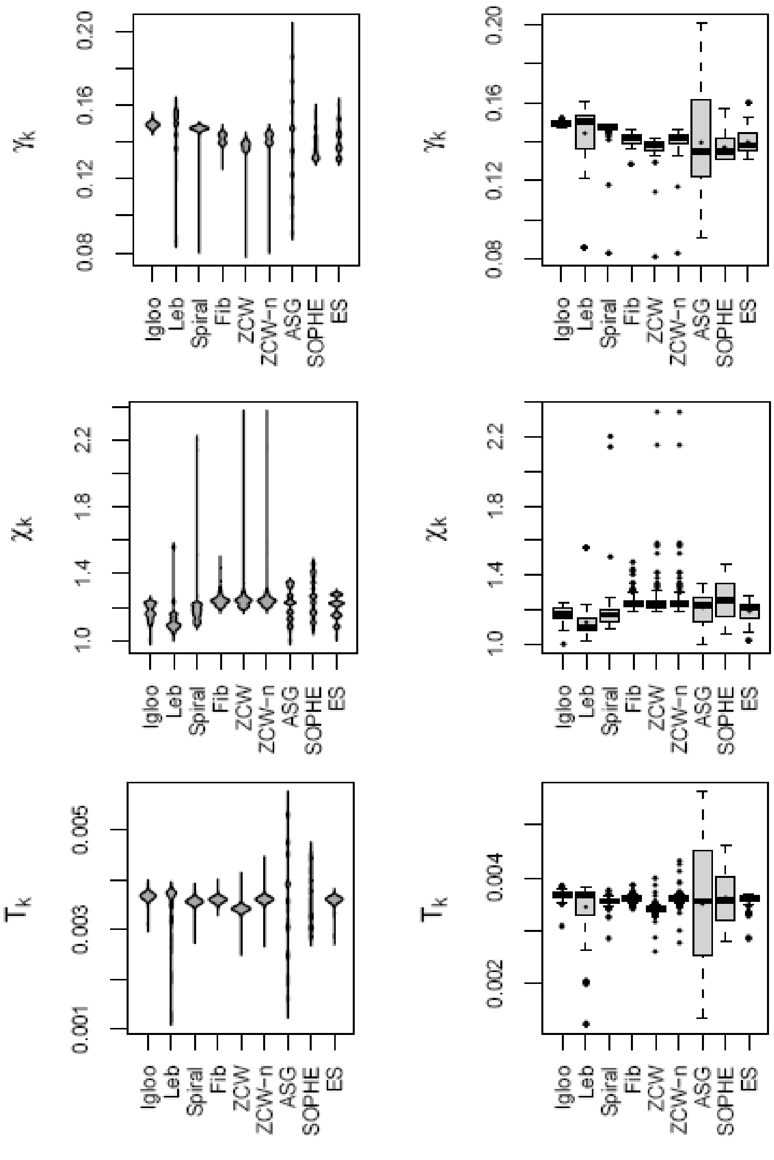

Fig. 1. The distributions of the γ_k , χ_k , and T_k quantities in beanplot (left) and boxplot (right) representation. The boxplots contain: boxes from the first to the third quartile of data (IQR); whiskers up to the most extreme points, but not further than 1.5IQR; a horizontal line inside the boxes for the median and a full knot for the mean value; open knots for the outliers [28].

Table 1. Statistical quantities for the distributions of the grids' geometric properties

Grid	γ_k			χ_k		
	median	range	IQR	median	range	IQR
Igloo	0.1493	0.0055	0.0012	1.1729	0.2409	0.0635
Leb	0.1502	0.0745	0.0174	1.0977	0.5383	0.0751
Spiral	0.1474	0.0642	0.0001	1.1720	1.1124	0.0762
Fib	0.1422	0.0175	0.0045	1.2371	0.2880	0.0323
ZCW	0.1385	0.0610	0.0034	1.2371	1.1598	0.0388
ZCW-n	0.1423	0.0629	0.0045	1.2369	1.1596	0.0327
ASG	0.1351	0.1104	0.0395	1.2259	0.3482	0.1373
SOPHE	0.1352	0.0261	0.0109	1.2559	0.4088	0.1886
ES	0.1383	0.0294	0.0086	1.2154	0.2602	0.0765

Grid	T_k [1]		
	median	range	IQR
Igloo	0.0037	0.0008	0.00007
Leb	0.0037	0.0026	0.00045
Spiral	0.0036	0.0009	0.00005
Fib	0.0036	0.0005	0.00004
ZCW	0.0034	0.0014	0.00003
ZCW-n	0.0036	0.0015	0.00004
ASG	0.0036	0.0043	0.00196
SOPHE	0.0036	0.0018	0.00083
ES	0.0036	0.0008	0.00006

[1] The statistical quantities are averages of the values obtained from three random samplings of the grids. For all grids, the ratio between the standard deviation and the mean for the three samplings was 0.01–0.05% for the median, 0.2–5.1% for the range, and 0.1–5.2% for IQR.

EasySpin and SOPHE have more distributed data, but a range which is more then twice smaller than for ZCW and ZCW-n.

b) The χ_k distributions for the Fibonacci, ZCW, and ZCW-n grids have the smallest IQR values. Nevertheless, the distributions for ZCW and ZCW-n present many outliers and have the highest range. The range is the smallest for Igloo, EasySpin, and Fibonacci grids.

c) The T_k distributions for the Fibonacci, EasySpin, Igloo, Spiral, ZCW, and ZCW-n grids have lower range and IQR values than for the Lebedev, SOPHE, and ASG grids. In case of SOPHE and ASG, the high IQR values indicate a wide spread of the T_k values within the whole range.

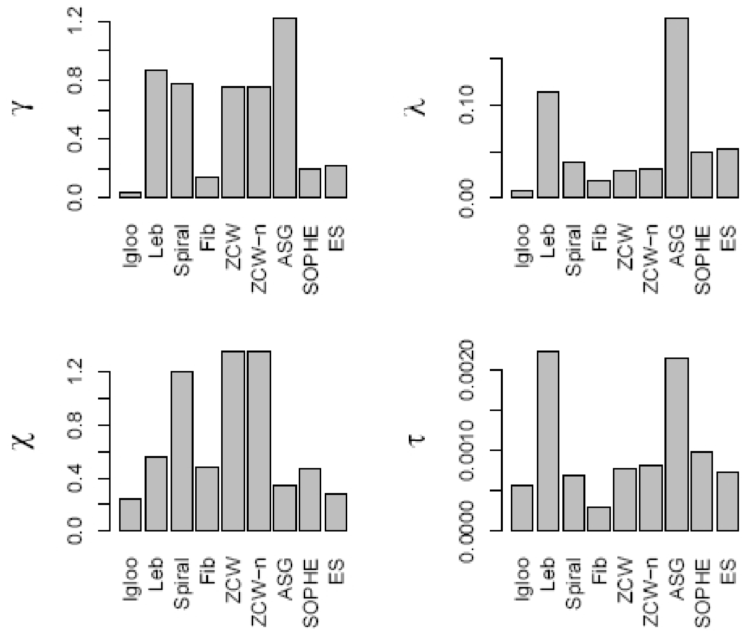

Fig. 2. The uniformity metrics

2. The uniformity metrics

The four metrics computed in this paper, which are global measures of the grids' uniformity, are presented in Figure 2. For each grid, the second moment trace measure τ is the average of the values obtained from three random samplings of the grid.

a) The mesh ratio values γ agree with the range values of the γ_k distributions (Table 1). According to γ, Igloo, Fibonacci, SOPHE, and EasySpin are the most uniform. The ZCW, ZCW-n, Spiral, and Lebedev grids have mesh ratio values between 5.5 and 6.4 times higher than the Fibonacci grid, while the ASG grid has a value about nine times higher.

b) The covariance measure λ differentiates less than the mesh ratio γ between the spiral-based grids Spiral, ZCW, and ZCW-n, on the one hand, and the triangular grids SOPHE and EasySpin, on the other hand. Based on covariance measure, Igloo and Fibonacci grids are the most uniform and the Lebedev and ASG grids the least.

c) Spiral, ZCW, and ZCW-n have the highest regularity measure χ, about 5–6 times higher than Igloo. From the four metrics investigated, the regularity measure is the single one for which the Lebedev and ASG grids present relatively small values.

d) The Fibonacci grid has the smallest second moment trace measure τ. The metric is 2–3.5 times higher for Igloo, Spiral, ZCW, ZCW-n, EasySpin, and SOPHE, and about 7.5 times higher for the ASG and Lebedev grids.

It should be noted that all uniformity metrics except the covariance measure λ depend on extreme values of some quantities calculated for the grid points or for the Voronoi cells of the grids. In some cases, the distributions of these quantities are characterised by relatively small IQR values, but present extreme outliers. This is the case, for example, for the χ_k and γ_k distributions of the Spiral, ZCW, and ZCW-n grids. Therefore, the distributions of the grids' geometric quantities characterise better the grids than the uniformity metrics, as already observed in [4].

The comparison of the grids according to the uniformity metrics and distributions is summarised in Table 2. The Fibonacci, Igloo, and EasySpin grids present low-range distributions and relatively small uniformity metrics in most cases. Moreover, the Fibonacci, ZCW, ZCW-n, Spiral, Igloo, and EasySpin grids have distributions with relatively low IQR values. As shown in reference [4], the Fibonacci, ZCW, ZCW-n, Spiral, and EasySpin grids do also generate low-noise simulated CW EPR powder spectra for some spin system symmetries.

Table 2. The spherical grids, in increasing order according to the uniformity metrics and the grids' geometric properties

Metric		**The grids' order**
γ_k	range	Igloo, Fib, SOPHE, ES, ZCW, ZCW-n, Spiral, Leb, ASG
	IQR	Spiral, Igloo, ZCW, ZCW-n, Fib, ES, SOPHE, Leb, ASG
γ		Igloo, Fib, SOPHE, ES, ZCW, ZCW-n, Spiral, Leb, ASG
λ		Igloo, Fib, ZCW, ZCW-n, Spiral, SOPHE, ES, Leb, ASG
χ_k	range	Igloo, ES, Fib, ASG, SOPHE, Leb, Spiral, ZCW-n, ZCW
	IQR	Fib, ZCW-n, ZCW, Igloo, Leb, Spiral, ES, ASG, SOPHE
χ		Igloo, ES, ASG, SOPHE, Fib, Leb, Spiral, ZCW, ZCW-n
T_k	range	Fib, Igloo, ES, Spiral, ZCW, ZCW-n, SOPHE, Leb, ASG
	IQR	ZCW, Fib, ZCW-n, Spiral, ES, Igloo, Leb, SOPHE, ASG
τ		Fib, Igloo, Spiral, ES, ZCW, ZCW-n, SOPHE, ASG, Leb

CONCLUSIONS

This paper has compared nine spherical grids used in magnetic resonance powder simulations, according to the following uniformity metrics: the mesh ratio, the covariance, the regularity, and the second moment trace measure. The metrics depend on geometric quantities, such as distances between the grid points or between points of the Voronoi cells. For each spherical grid, these quantities have some distribution on the unit sphere. Three out of four investigated metrics depend only on the distributions' extreme values, which may be some outliers. Therefore, the distributions of the grids' geometric properties are better measures of the grids' quality than the global uniformity metrics.

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