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ON THE INFLUENCE OF THE INTERACTION LAWS OF A DYNAMICAL
PARTICLE SYSTEM FOR SAMPLE OPTIMIZATION

Abstract

The presented paper investigates the effect of the formulation of the energy potential of a dynamical particle system used for the optimization of statistical point sampling. The dynamical particle system, originally developed as a physical analogy to the Audze-Eglajs (AE) optimization criterion and its periodical modification (PAE), effectively demonstrated that the originally proposed energy potential performs well only in poorly applicable scenarios featuring low-dimensional design domains filled with a rather high number of design points. A remedy is presented which involves a refined formulation of the energy potential, as well as its derivation. The reasoning behind this approach is also dealt with in detail.

Keywords

Particle dynamical system, statistical sampling optimization, periodic space, particle interaction laws, short- and long-range interactions, self-similar designs.

1 INTRODUCTION

Monte-Carlo type numerical integration requires the sampling of integration points that are distributed uniformly throughout a design domain with respect to probabilities. The layout of the design points crucially affects the performance of this type of numerical integration. The use of an ideally distributed set of integration points is also of interest in many other engineering and research fields. While sampling from a random vector or integrating an unknown function, using a uniform integration point layout is the only possible way to minimize the lower bound of the resulting error. We consider the design domain to be a unit hypercube $[0,1]^{N_{\text{var}}}$, where N_{var} is the number of variables (dimension) and the desired distribution inside the hypercube is uniform.

However, “uniformity” is not a recognized property of a sampling point distribution. Many criteria have been proposed in recent years for the evaluation of the uniformity of point layouts (or *sampling plans*) containing N_{sim} points within the design space of a specific dimension N_{var} . Typically, these criteria investigate point layouts with a tendency to prefer designs with points distributed so that they are equally distant from each other. Certain criteria are derived from analogies with physical problems.

The Audze-Eglajs (AE) criterion [1], in particular, may be considered an elegant instance of such criteria. Its objective is the minimization of the potential energy of a system of mutually repelling particles. With their positions, these particles represent the positions of sampling points within a unit hypercube design domain. In recent years it has been proposed that the original Audze-Eglajs criterion suffers from the existence of design space boundaries [2, 3]. A remedy for this

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behavior was also proposed [2, 3]. It assumes a periodically extended design hypercube, in the case of which the boundaries naturally disappear. Building on such a refined Periodic Audze-Eglajs criterion (PAE), it has been proved that usage of the PAE criterion leads to designs that are statistically uniform (from design to design) and to a well distributed set of points for every single point layout.

2 AUDZE-EGLAJS AND PHI CRITERIA

The original formulation of the AE criterion [1] (see also [4, 5, 6, 7]) considers the analogy between the sampling plan and a system of charged particles with repulsive forces. The potential energy of the system is the sum of energies $1/L_{ij}^2$ accumulated by each pair of points i and j . Instead of the sum of energies, one can alternatively calculate the average potential energy, i.e. divide the total energy by the number of pairs of points, $N_p = \binom{N_{\text{sim}}}{2}$. The AE criterion then reads:

$$E_n^{\text{AE}} = \frac{1}{N_p} \sum_{i=1}^{N_{\text{sim}}-1} \sum_{j=i+1}^{N_{\text{sim}}} \frac{1}{L_{ij}^2}, \quad (1)$$

where L_{ij} is the inter-site Euclidean distance between points i and j depends on the Cartesian coordinates of said points, $\mathbf{x}_i = \{x_{i,v}\}$, $i = 1, K, N_{\text{sim}}$, $v = 1, K, N_{\text{var}}$:

$$L_{ij} = \sqrt{\sum_{v=1}^{N_{\text{var}}} (\Delta_{ij,v})^2}, \quad (2)$$

where:

$$\Delta_{ij,v} = |x_{j,v} - x_{i,v}|, \quad (3)$$

is the projection of the distance L_{ij} onto the axis v .

A generalization of the AE criterion is the ϕ criterion [8]:

$$\phi_{(d,\lambda)} = \left(\frac{1}{N_p} \sum_{i=1}^{N_{\text{sim}}-1} \sum_{j=i+1}^{N_{\text{sim}}} \frac{1}{d^\lambda(\mathbf{x}_i, \mathbf{x}_j)} \right)^{\frac{1}{\lambda}}. \quad (4)$$

This criterion considers a general power, λ , of the distance (metric) d . The combination of $\lambda = 2$ and the Euclidean inter-site distance d makes $\phi_{(d,\lambda)}$ identical to the AE criterion. As $\lambda \rightarrow \infty$, the criterion increasingly prioritizes designs where the minimal distances are maximized, which is, in limit, the Maximin distance criterion [9]. Using the analogy with the system of charged particles, one can say that with increasing power λ a greater portion of energy is stored in short-range interactions.

The power $1/\lambda$ upon the entire sum is, in fact, a monotonous transformation (the difference between designs is not distorted) and can be dropped as well. Therefore, a simplified version of the criterion with the parameters of a used metric $d(\mathbf{x}_i, \mathbf{x}_j)$ and exponent value λ may be considered:

$$\phi_{(d,\lambda)} = \frac{1}{N_p} \sum_{i=1}^{N_{\text{sim}}-1} \sum_{j=i+1}^{N_{\text{sim}}} \frac{1}{d^\lambda(\mathbf{x}_i, \mathbf{x}_j)}. \quad (5)$$

The standard way of measuring the inter-point distances is the Euclidean length defined above in Eq. (2): $d(\mathbf{x}_i, \mathbf{x}_j) = L_{ij}$. It has been shown that due to the presence of the boundaries of the design domain, the metric used in the criteria Eq. (1,4,5) leads to a non-uniform point distribution [2,3,10]. Moreover, the authors of [2,3,10] have shown that if the metric $d(\mathbf{x}_i, \mathbf{x}_j)$ is modified so that it considers distances measured in the periodically repeated design domain (a *periodic metric*), the criterion becomes invariant with respect to arbitrary shifts along individual dimensions. A simplified

version of the periodic space considers only the shortest distances, i.e. the distance is taken as $d(\mathbf{x}_i, \mathbf{x}_j) = \bar{L}_{ij}$, where \bar{L}_{ij} is the Euclidean distance between the i -th point and the closest image of the j -th point within the periodic space:

$$\bar{L}_{ij} = \sqrt{\sum_{v=1}^{N_{\text{var}}} (\bar{\Delta}_{ij,v})^2}, \quad (6)$$

where:

$$\bar{\Delta}_{ij,v} = \min(\Delta_{ij,v}, 1 - \Delta_{ij,v}) \quad (7)$$

is the shortest projection of the distance between points i and the nearest image of j onto axis v .

Using this definition of distance, Eq. (5) reads:

$$\phi_{(\bar{L}, \lambda)} = \frac{1}{N_p} \sum_{i=1}^{N_{\text{sim}}-1} \sum_{j=i+1}^{N_{\text{sim}}} \frac{1}{\bar{L}_{ij}^\lambda}. \quad (8)$$

Utilizing the above-described nomenclature, the AE criterion can be denoted as $\phi_{(L, 2)}$. The periodic version of the AE criterion (the PAE criterion [2]) uses a combination of exponent $\lambda=2$ and the shortest (periodic) metric \bar{L}_{ij} , and therefore can be denoted as $\phi_{(\bar{L}, 2)}$.

The authors of [2] argue that even for exponent as small as $\lambda=2$, the consideration of the shortest distance \bar{L}_{ij} suffices to deliver invariance with respect to random shifts along individual dimensions and thus prioritizes designs leading to statistical uniformity of coverage. Moreover, it is argued that the shortest distance is the one associated with the highest contribution to the criterion. As a result, the PAE criterion captures the important features of the full periodic repetition of the design space. The next section generalizes the criterion in Eq. (8) by considering a higher number of copies of the design domain.

3 PERIODIC EXTENSION OF THE DESIGN DOMAIN

In this section we consider a generalized model in which a certain number of periodic repetitions of the original design domain are considered. Using the nearest image of point j with respect to point i , as considered in Eq. (8), does not cover a true periodic repetition of the design domain. We argue that the above-presented approach is a simplification that can be shown to yield identical results to the fully repeated system in the case of a sufficient point count N_{sim} . If the number of points in the original system is too small to carry enough information about the pattern of a periodically repeated system, making a periodic extension to a sufficient level is desirable.

In a true periodic domain, an infinite number of images of point j would interact with point i . When a finite number of copies of the design domain are considered, not only the *real* particle j , but also all periodically repeated images of the particle j will contribute to the potential:

$$\phi_{(\bar{L}, \lambda, k_{\text{max}})} = \sum_{i=1}^{N_{\text{sim}}-1} \sum_{j=i+1}^{N_{\text{sim}}} \left(\frac{1/N_p}{\bar{L}^\lambda(\mathbf{x}_i, \mathbf{x}_j)} + \sum_{k=1}^{k_{\text{max}}} \sum_{c=1}^{c_{\text{max}}} \frac{1/N_p}{L^\lambda(\mathbf{x}_i, \mathbf{x}_j + \mathbf{s}_c)} \right), \quad (9)$$

where k_{max} , which has been introduced as an additional parameter, is the number of added periodical extensions (envelopes) of the space. In the fully repeated system $k_{\text{max}} = \infty$, and analogically, for a non-extended system $k_{\text{max}} = 0$. Therefore $\phi_{(\bar{L}, \lambda)} \equiv \phi_{(\bar{L}, \lambda, 0)}$: compare Eqs. (8) and (9).

When a certain number of envelopes k_{max} are considered, the number of copies of the design domain is denoted as c_{max} . The vector \mathbf{s}_c is the vector needed to shift the original point \mathbf{x}_j to the

particular periodically repeated version indexed by c . The distances to the periodically repeated images of point j must be measured as standard Euclidean distances.

A single “level” of periodic extension adds another envelope of periodically repeated images of all other particles around each point (see Fig. 1 and 2e). Such an extension provides additional information about the point layout within the domain.

The level of the periodic extension is quantified by a positive integer k_{\max} . Within an extended periodic domain of finite value of k_{\max} , particle i interacts not only with the actual particle j , but also with all of the $c_{\max} = \left[(2k_{\max} + 1)^{N_{\text{var}}} - 1 \right]$ images of particle j as well (see Fig. 1 for $N_{\text{var}} = 1$). The envelopes are considered to be centered around the shortest distance with \bar{L}_{ij} .

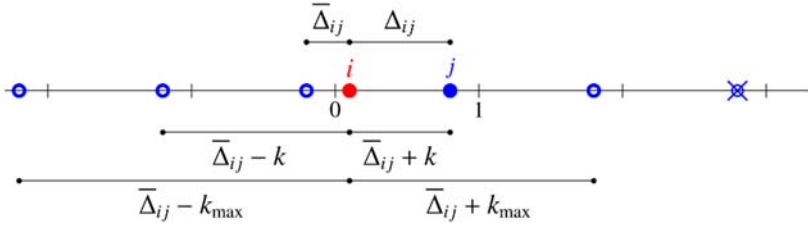


Fig. 1: 1D example of the periodic extension of level $k_{\max} = 2$.

4 THE EXPONENT λ

This section focuses on the exponent λ in the periodic ϕ criterion [10] (see Eq. (8)). In the original AE criterion and also in the periodic version (PAE), the potential energy between each pair of points is not dependent on the dimension, N_{var} . It has been found [12] that the character of the criterion is different for various N_{var} and also for various numbers of points, N_{sim} . In the 1D situation, the energy tends to infinity *linearly* with increasing N_{sim} . In 2D ($N_{\text{var}} = 2$), the energy tends to infinity as $\ln(N_{\text{sim}})$, which is not a power law. For dimensions $N_{\text{var}} \geq 3$, the energy tends to a constant for increasing N_{sim} . This behavior can be explained by the fact that for a given $N_{\text{var}} > 1$, various numbers of points lead to different proportions between energy due to the *long-range* and *short-range* interactions. The higher the number of points, the higher the proportion of energy stored in long-range interactions. This may not be desirable behavior as the criterion becomes insensitive to local clusters of points in high dimensions and also with high numbers of points: it becomes dominated by long-range interactions.

It is suggested that the power be at least $\lambda = N_{\text{var}} + 1$. With this power, the interaction is *dominated* by *short-range* interactions. With such a sufficient exponent λ , the convergence of the potential energy $\phi_{(L,\lambda)}$ or better $\phi_{(\bar{L},\lambda)}$ towards infinity for a uniform distribution of points is a *power law*. Such a convergence signals the self-similarity of the problem or the absence of a length scale. In other words, a zoom into a sufficiently dense uniform design with a window greater than a certain size (see below) carries all features of the full design and has an energy value which can be easily scaled from the value corresponding to the smaller zoom.

This can be shown by studying the behavior of the radial part of the integral of the potential over the volume V of the given N_{var} -dimensional domain. The potential energy for a uniform design reads:

$$I = \int_{N_{\text{var}}} \frac{1}{L^\lambda} d^{N_{\text{var}}} V, \quad (10)$$

where L is used to denote the one-dimensional distance between points (the symbol d is not used, as this will avoid confusion with the symbol d that is used to denote the differential). Transforming this into polar coordinates gives:

$$I = \int_{N_{\text{var}}} \varphi d^{N_{\text{var}}} V |J| \frac{1}{L^\lambda} dL, \quad (11)$$

where $|J|$ is the Jacobian. The volume element is thereby given as:

$$d^{N_{\text{var}}} V = L^{N_{\text{var}}-1} dL \cdot d\varphi \prod_{i=1}^{N_{\text{var}}-2} \sin^{N_{\text{var}}-1-i}(\varphi_i). \quad (12)$$

Therefore, the integral is performed over the product $L^{N_{\text{var}}-1-\lambda}$. Performing just the radial integration leads to:

$$I_r = \int \frac{L^{N_{\text{var}}-1}}{L^\lambda} dL = \int L^{N_{\text{var}}-1-\lambda} dL. \quad (13)$$

For $\lambda=2$ as used in the AE criterion, we get the behavior described above. Using $\lambda = N_{\text{var}}$ leads to:

$$I_r = \int L^{-1} dL = \ln(L), \quad (14)$$

which diverges logarithmically; the interaction is still *long-ranged*.

Using $\lambda = N_{\text{var}} + 1$ yields:

$$I_r = \int L^{-2} dL = \frac{1}{L}, \quad (15)$$

which has the desired asymptotic behavior dominated by short-ranged interactions. Using powers $\lambda > N_{\text{var}} + 1$ only increases the (asymptotically constant) ratio between short-range and long-range interactions.

Fig. 2 shows the convergence of the normalized potential energy $\phi_{(\bar{L}, \lambda)}$ with the rise in the number of particles, N_{sim} . Instead of presenting the results for the point count, N_{sim} , we introduce a variable l_{char} , the *characteristic length*, a variable that involves also the dimension of the space. The characteristic length is defined as:

$$l_{\text{char}} = \frac{1}{N_{\text{var}} \sqrt{N_{\text{sim}}}}. \quad (16)$$

It can be seen that with the original exponent value $\lambda=2$ in the dimension $N_{\text{var}}=2$ ($\lambda=N_{\text{var}}$), the potential energy of the system does not converge to a power law but instead diverges logarithmically (roughly $\phi_{(\bar{L}, \lambda)} \approx \pi \ln(N_{\text{sim}}) + 1/\sqrt{N_{\text{sim}}} - 1/N_{\text{sim}}$). In higher dimensions of $N_{\text{var}} \geq 3$, the exponent $\lambda=2$ further leads to the convergence of the potential energy to a constant [12].

Using the above-proposed exponent $\lambda = N_{\text{var}} + 1$, the potential energy value tends to a power law as $N_{\text{sim}} \rightarrow \infty$:

$$\phi_{(\bar{L}, N_{\text{var}}+1)} \propto \frac{1}{l_{\text{char}}}. \quad (17)$$

Such behavior is desired as the designs for a given dimension N_{var} tend to have a universal self-similar pattern and the dependence on sample size disappears (no length scale is present). Thus the character of the criterion is kept independent of N_{sim} and the ratio between short-range interactions and long-range interactions is constant. This stabilization is obtained for a sufficient number of points within the design domain (a kind of tile). The self-similarity is manifested by the power law dependence (a straight line in Fig. 2). When the exponent is taken even higher ($\lambda > N_{\text{var}} + 1$), the self-similar regime is achieved for an even smaller number of points (greater l_{char}).

The graphs in Fig. 2 suggest that there must be link between (a) the exponent (responsible for the ratio between long- and short-range interactions) and (b) the number of “dummy” copies of the design domain that also modify the proportion of iterations of each type. This aspect is discussed in the next section.

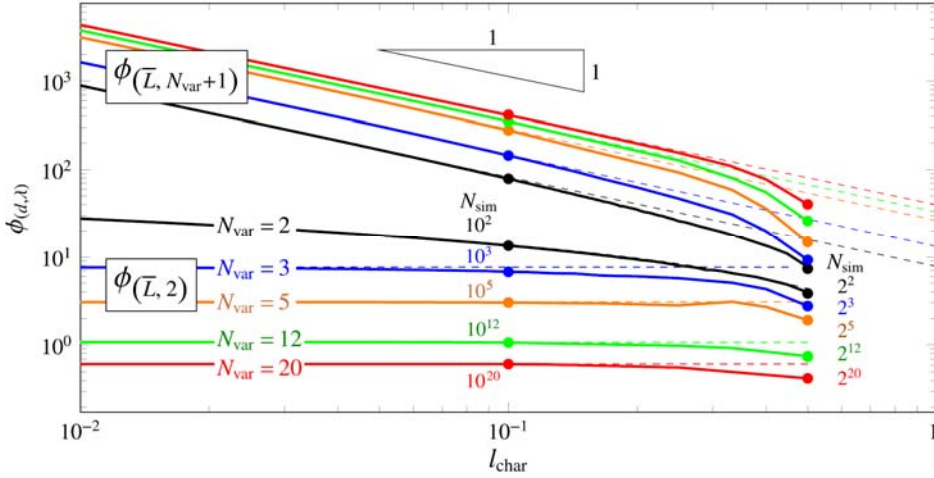


Fig. 2: Convergence of the normalized potential energy $\phi_{(\bar{L},\lambda)}$ depending on the exponent λ . The coloring that designates N_{var} is identical for the two bundles of curves. Solid circles are accompanied by the sample count corresponding to the l_{char} and N_{var}

5 ON THE SEEMINGLY SIMILAR EFFECT OF RAISING THE EXPONENT λ AND INCREASING THE LEVEL OF PERIODIC EXTENSIONS

Let us consider a few-body ($N_{\text{sim}} = 3$) particle system in the design space of $N_{\text{var}} = 2$ while using a potential with the exponent $\lambda = 2$. When considering the point layout via the $\phi_{(\bar{L},\lambda)}$ interaction, only two mutual distances to other points exist for each point, i.e. there are two forces acting upon each particle.

With an exponent of such insufficient magnitude, these forces do not differ significantly enough to correctly represent which particle shall be considered to be close (short-range interaction) or distant (long-range interaction). Raising the exponent above a certain threshold (discussed above) does lead to the needed qualitative change in the ratio between the acting forces: the closer particles start to act as short-ranged while the more distant particles remain long-ranged. In fact, the higher the exponent, the larger the portion of potential energy that will be stored in the short-range interactions.

The analogy between the effect of increasing the number of envelopes in $\phi_{(\bar{L},\lambda,k_{\text{max}})}$ and raising the exponent in $\phi_{(\bar{L},\lambda)}$ is evident. While using the original (low) value of the exponent λ , the majority of the potential energy is stored in the long-range interactions. However, the number of particles is not sufficient for the criterion to distinguish between short and long range. All particles seem to be at similar distance from one another as the design is not filled enough.

The $\phi_{(\bar{L}, \lambda, k_{\max})}$ interaction adds one or more additional envelopes of neighboring images of actual particles. These images, naturally, will act as long-ranged. The range is even greater than that of the real particles previously acting as long-ranged. This leads to a qualitatively more accurate distribution of the forces acting upon the real particles. Hence the identical behavior of the $\phi_{(\bar{L}, \lambda, k_{\max})}$ and the $\phi_{(\bar{L}, \lambda)}$ when in interaction with a correct exponent:

- the $\phi_{(\bar{L}, \lambda, k_{\max})}$ interaction does add long-range points so that the actual particles seem closer,
- the $\phi_{(\bar{L}, \lambda)}$ interaction with the corrected exponent changes the ratio between the forces so that the close particles seem closer and the distant particles seem more distant.

It can therefore be shown that while simulating a few-body problem with the $\phi_{(\bar{L}, \lambda)}$ interaction, it is advisable to raise the exponent λ even above the lower bound of $N_{\text{var}} + 1$ in order to force the desired self-similarity for various N_{sim} .

When using the $\phi_{(\bar{L}, \lambda, k_{\max})}$ interaction, especially for few-body problems, the greater context of the pattern is carried within the interaction as $3^{N_{\text{var}}}$ images of each particle are considered there. Effectively, a system mimicking $N_{\text{sim}} \cdot 3^{N_{\text{var}}}$ particles is being simulated and an identical pattern should be obtained (see Fig. 3b and 3f).

On a side note, the simulation of a greater (extended) system might be a slower option compared with the correction of the exponent in the energy potential. This is because the number of additional points within the envelopes rises steeply.

6 COMPUTER IMPLEMENTATION

The simulation of a particle system is typically a computationally demanding task. However, it is possible and beneficial to conduct the implementation of the solution in a manner that is as parallel as possible. The degree to which parallelism can be achieved dominantly depends on the nature of the problem at hand, and also on the capabilities of the hardware used. The implementation of the solution of the proposed dynamical particle system was conducted using the nVidia CUDA platform.

The equations of motion of the dynamical particle system contain independent accelerations on the left-hand side. This means that accelerations of particles can be solved separately without solving a system of equations. Furthermore, the computation of the mutual distances as well as the numerical integration of equations of motion using the semi-implicit Euler method can be conducted in parallel.

The derivation of equations of motion, and the nature of the implementation and speed-up, are not trivial and have already been covered in detail in concurrent publications [13, 3].

7 RESULTS OF NUMERICAL SIMULATIONS

The following section presents examples of numerical simulations of the dynamical particle system, mainly focusing on the effect of the value of the exponent λ in the energy potential as well as on the effect of periodical extension.

To start off, let us show how the ability of a self-similar design (power-law quality) disappears while the number of particles N_{sim} decreases. In a design space of dimension $N_{\text{var}} = 2$, the original exponent value $\lambda = 2$ only yields an ideal distribution if the design space is filled enough. For $N_{\text{var}} > 2$, the original exponent leads to primitive (and even incomplete) ortho-grid patterns.

Studying the design space of dimension $N_{\text{var}} = 2$, Fig. 3a, 3b and 3c show that an ideal triangular grid pattern (if possible) is reached as long as the information needed to create such a self-similar pattern is provided (the number of points is sufficient). When the number of particles becomes insufficient, the interaction is not approximated well enough (in pursuit of a perfect triangular grid) and then primitive (even incomplete) ortho-grids are produced (see Fig. 3d).

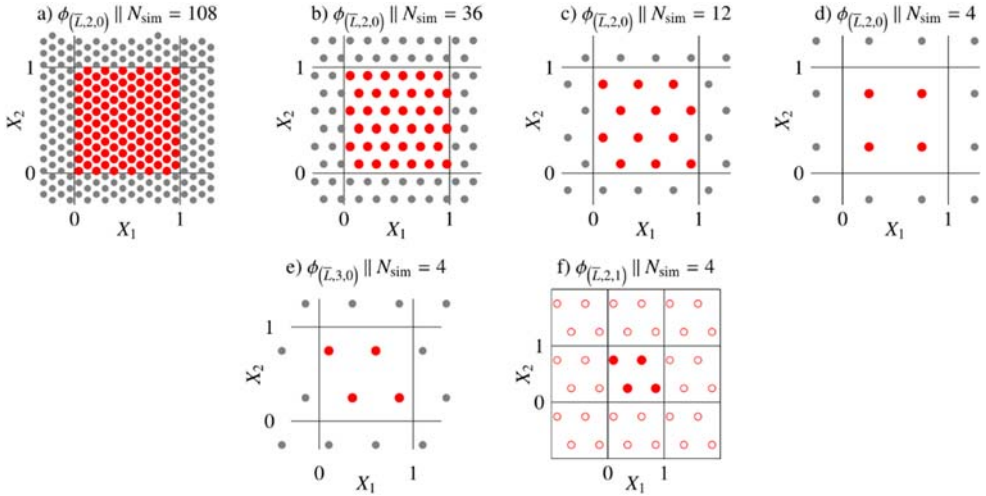


Fig. 3: Disappearance of the quality of a self-similar design as yielded by the original PAE formulation, and the effect of remedies proposed.

A remedy, as described above, can be effected via two seemingly dissimilar approaches. First, see Fig. 3e for an example of a layout obtained with an exponent λ with a sufficiently high value. Second, the result of a simulation using a periodic extension of a single envelope ($k_{\max} = 1$) is provided. Such a simulation effectively considers $4 \cdot 3^2 = 36$ points (4 of which are actual particles) (see Fig. 3f). Hence, the entire extended space is filled equivalently to that of the non-extended ($k_{\max} = 0$) simulation of 36 particles (see Fig. 1b). An identical point layout of 36 points is therefore achieved and, in a way, the resulting layout for the system of $N_{\text{sim}} = 4$ is cut out of a greater scenario.

It is worth noting that, when simulating such an extended system (36 particles instead of 4 particles), the power-law quality is easier to achieve as the higher theoretical N_{sim} (lower l_{char} value) occurs closer to the power-law asymptote (see Fig 2).

Another portion of simulation examples concerns the results of simulations within a three-dimensional design space ($N_{\text{var}} = 3$). For this and higher dimensions, the original formulation of the (P)AE potential already malfunctions and yields poor designs based dominantly on ortho-grids (see Fig. 4a). The result of the remedy of raising the value of the exponent λ is provided (see Fig. 4b).

Such a refined formulation of the energy potential, we believe, will lead to perfect designs not only within the design space of the complete dimension, but also in all sub-spaces of a lower dimension (see Fig. 4).

A question may arise whether the designs obtained using the dynamical simulation of a particle system with the proposed criteria cover the design domain uniformly. The authors understand uniformity in two different ways: statistical uniformity of many designs and uniformity within a single design. The statistical uniformity, i.e. the equal probability of any point from the design domain to be selected, is fulfilled inherently due to the invariance of the criteria with respect to translations along any dimension, see [2]. Regarding the uniformity of point distribution within a single design, this quality is inherently fulfilled due to the formulation of potential energy: the repulsive forces between all pairs of particles guarantee that there are no clusters contained in configurations of global minima and the points are scattered “uniformly” over the design domain.

The uniformity requirement is motivated by the need to perform integral estimations using Monte-Carlo sampling. Samples obtained by the proposed method provide accurate estimations of integrals with a small variability. A comparison of integral estimates with other known techniques is provided in depth in [11].

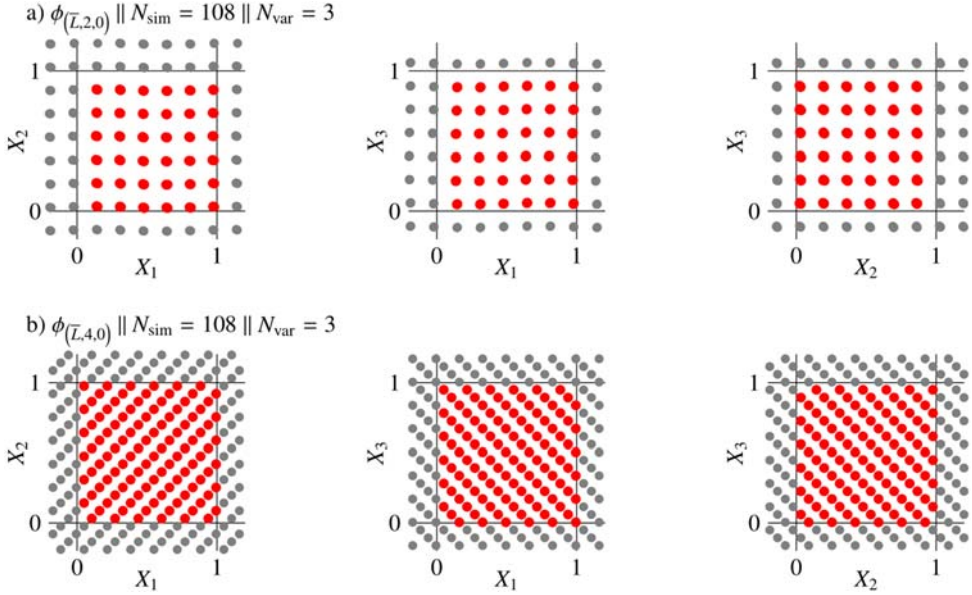


Fig. 4: 3D designs: a) the original PAE ($\lambda = 2$), b) the corrected potential exponent ($\lambda = N_{\text{var}} + 1$).

8 CONCLUSION

The paper investigates the formulation of the energetic potential of the Audze-Eglajs optimization criterion and its periodical modification PAE. Remedies for the incorrect behavior of systems with low numbers of particles and high dimensions are proposed.

An indirect solution that provides appropriate few-body system layouts lies in simulating a greater scenario: the consideration of additional envelopes of the periodically repeated system. In this way, richer information about the pattern is provided and the optimal point layout can be obtained. However, such a scenario mimics the simulation of a system with a higher number of particles and does not lead to the correction of the malfunctioning energy potential.

An overarching remedy was therefore pursued, leading to a potential which takes into account the dimension of the problem, N_{var} . First, a generalization of the potential based on the ϕ criterion is provided so the crucial parameters of the potential, the metric d and the exponent λ , can become the subject of refinement.

Further derivation was based on the desire for the ability to create self-similar patterns of point layouts for various point counts. With the proposed value of the exponent λ , the convergence of the potential energy of the criterion towards infinity for a uniform distribution of points is a power law. Such a convergence signalizes the self-similarity of the problem or the absence of a length scale. Using such a refined interaction, optimal (self-similar) designs are produced even for scenarios of arbitrary dimension, N_{var} , or few-body systems, as was shown.

In this way, the role of the exponent featured in the phi criterion is explained using an analogy with a system of repulsive particles.

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