# Estimation of Fekete Points

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**Abstract**

In this paper we present a new method to estimate Fekete points on surfaces. Although our method works in a general setting, we concentrate on its application to the unit sphere because it is the prototype problem and in the unit cube because its singularity. The algorithm we present here is very simple and it is based in a physical interpretation of the behavior of a system of particles when they search for a minimal energy configuration. Moreover, the algorithm is efficient and robust independently of the surface and the kernel used to define the energy. The algorithm allows us to work with a great number of particles, for instance, in less than a day of calculation time, we have obtained a good configuration for 50000 particles in the unit sphere without using symmetry properties and with a conventional PC.

## 1 Introduction

The problem of obtaining Fekete points in a manifold fills a pre-eminent place in the mathematical research of the last decades. In its original version, the problem consists in determining the position of $N$ points on a compact subset $S \subset \mathbb{R}^2$ that maximize the product of their mutual Euclidean distances. The $N$-tuples, $\omega_N = \{x_1, \ldots, x_N\}$, that satisfy the above property are the so-called *$N$-th order Fekete points* in $S$. It is not difficult to check that those $N$-tuples minimize in $S$ the functional

$$\mathcal{I}(\omega_N) = \sum_{1 \leq i < j \leq N} \mathcal{K}(x_i, x_j), \tag{1}$$

where $\mathcal{K}(x_i, x_j) = -\ln |x_i - x_j|$ is the so-called *logarithmic kernel* and $|x_i - x_j|$ is the Euclidean distance between $x_i$ and $x_j$. The value $\mathcal{I}(\omega_N)$ represents the *potential energy* corresponding to the logarithmic kernel when an unitary weight is associated with any point. In the three-dimensional Euclidean space multiple variants of the problem can be formulated by considering different kernels, among which the *Riesz's kernels*, defined as $\mathcal{K}(x_i, x_j) = |x_i - x_j|^{-s}$ with $s > 0$, constitute a family of special interest. In particular, the *Newtonian kernel*,

obtained taking $s = 1$, has became the most relevant case and its potential energy $\mathcal{I}(\omega_N)$ is named *electrostatic potential energy*. For a more detailed description of this topic, see for instance [7].

The determination of Fekete points in the unit sphere is considered as a model of a highly non-linear optimization problem with non-linear constraints. In fact, obtaining a robust and efficient algorithm for that problem still constitutes a challenge in computational mathematics [13]. In general, only when the constrains are linear or they can be sufficiently well approximated by linear constrains it is reasonable to expect a good behavior of the usual algorithms for optimization problems with constrains. But, even in this case, the convergence ratios result lower than the corresponding to free optimization methods. Some authors choose to transform problems as the Fekete points one in optimization problems without constrains by considering a parametrization of the surface [8, 16]. In this way, they can use classical optimization techniques such as the *Gradient Method*, the *Conjugate Gradient Method*, the *Newton Method* and the family of *quasi-Newton methods*. Also other methods like the so-called *Combinatory Optimization methods* have been used, among which they stand out the *Simulated Annealing*, *Tabu Search* and *Genetic Algorithms* [8].

A considerable amount of theoretical and numerical results have been obtained in relation with the different versions of Fekete points problem, see for instance [5, 6, 8, 10, 11, 14, 16], and it has been completely solved in some particular cases. Nevertheless, recent publications recognize that the simple obtaining of a position near to a local optimum for hundreds of points in the sphere requires to make use of an important calculation infrastructure. Moreover, they raise the possibility of obtaining good configurations of thousands of points reducing the number of unknowns by means of symmetries, see [4].

The resolution of this kind of problems has a lot of theoretical and practical implications in areas as Mathematics, Chemistry, Biology, Numerical Computation (interpolation schemes, FEM meshes, numerical integration) and CAD, see for instance [1, 2, 8, 11, 14, 16].

# 2 The Method

We present here the basis of an algorithm for the obtaining of Fekete points in a surface. We consider that the results obtained with this algorithm are highly satisfactory. For instance, in less of a day of calculation time, we have obtained good configurations for 50000 points in the unit sphere without using symmetry properties and with a conventional Pentium IV processor of 2.54 GHz and 512 Mb of RAM. The objective of this paper is not to mark the limits of applicability of the algorithm but to introduce the main ideas on which it is based, to establish its extraordinary simplicity and to analyze its numerical behavior. For this reason all the calculations presented in this work have been carried out with the above mentioned processor. The algorithm has a good behavior independently of the kernel and the surface considered. In that sense, we present its application to two surfaces: the unit sphere, because it is the most treated problem in the literature related with the estimation

of Fekete points, and the unit cube, because of the difficulty that represent its singularities in the edges and in the vertices. The basic structure of the algorithm is classical, in the sense that each iteration consists on obtaining the advance direction and the step size in a deterministic way.

The ideas behind the algorithm come from Physics. We do not try to answer directly the question about which are the minimum potential energy configurations, but how the points of a non-optimal configuration can advance, in a mechanical sense, to reach a minimum potential energy configuration. The equivalence between minimum potential energy and static stable equilibrium configurations constitutes the key of the method. A mechanical system formed by particles is in equilibrium if the total force that acts on each one of these particles is null. The equilibrium is stable if small perturbations in the position tend to return each particle to its original position, and then this position is a minimum for the potential energy of the system. So, for a given non-optimal configuration, non-equilibrated forces must act on the particles, and these forces will inevitably induce its movement. We wonder about the character of these forces and this movement and when it will carry the particles to an equilibrium position [3].

Firstly note that the energy of a system of $N$ particles, $x_k \in \mathbb{R}^3$, $k = 1, \ldots, N$, is given by $\mathcal{I} = \dfrac{1}{2}\sum_{i=1}^{N} V_i$, where $V_i = \sum_{\substack{j=1 \\ j\neq i}}^{N} \mathcal{K}(x_i, x_j)$ is the potential created on $x_i$ for all the other particles. The problems we are interested in, require that all the particles lye on a regular surface $S \subset \mathbb{R}^3$, in such way that any point $x_i \in S$ has assigned a normal vector $n_i$. If we fix the position of the $N-1$ particles $\{x_j \in S : j = 1, \ldots, N, j \neq i\}$, $V_i$ is a function of $x_i$ and the opposite of its gradient, that we will denote by $F_i = -\nabla V_i \in T_{x_i}(\mathbb{R}^3)$, represents the repulsive force that acts on the $i$-th particle due to the existence of the rest. We will consider $F_i^n = \langle F_i, n_i\rangle n_i$ and $F_i^T = F_i - F_i^n$, the *normal and tangent components* to $S$ of the force $F_i$ at $x_i$, respectively. On the other hand, if $M = S^N$, then $\left(F_1^T, \ldots, F_N^T\right) = -\nabla \mathcal{I}_{|M}$ is the direction of maximum descent of $\mathcal{I}$ in $M$, independently of the possible parametrizations of $S$.

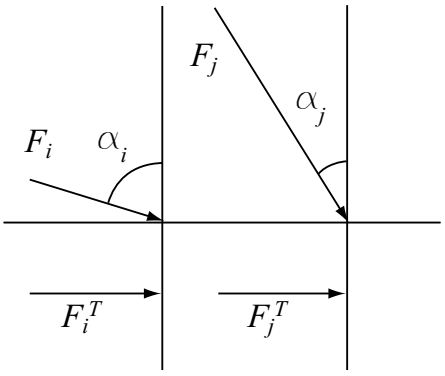


Figure 1: Disequilibrium degree

The $i$-th particle is in *equilibrium* on $S$ if $F_i^T = 0$. Therefore, $|F_i^T|$ could be a measure

of the disequilibrium degree of that particle on $S$. Nevertheless, Fig. 1 suggests that an alternative measure of disequilibrium degree based on the angle between $F_i$ and $n_i$ could result more satisfactory. In effect, two particles $x_i, x_j$ with $|F_i^T| = |F_j^T|$ can be "more or less equilibrated" on $S$ depending on the angle between the forces $F_i$ and $F_j$ and its corresponding normal vectors $n_i$ and $n_j$. We define $\dfrac{|F_i^T|}{|F_i|}$ as the *disequilibrium degree* of the $i$-th particle. The suitability of this election will be showed clearly throughout the paper.

The following simple proposition establishes that to advance according with this disequilibrium measure descents the energy of the system.

**Proposition 2.1** *The direction*

$$w = \left( \frac{F_1^T}{|F_1|}, \ldots, \frac{F_N^T}{|F_N|} \right)$$

*is of descent of the energy constrained to $M$. In addition, every particle contributes to the descent.*

**Proof.** The direction $w$ is obviously compatible with the constraints of the problem, since $w \in T_x(M)$. The result follows from the fact that

$$\langle w, -\nabla I_{|M} \rangle = \sum_{i=1}^{N} \frac{|F_i^T|^2}{|F_i|} \geq 0. \quad \blacksquare$$

Observe that the direction $w$ does not coincide with the one given by the Gradient method except in very particular cases, for example in the sphere with a great number of particles when they are in stages very close to the equilibrium. The rest of classical optimization methods, as Conjugate Gradient, Newton or quasi-Newton, choose advance directions that in general do not guarantee that each particle contributes to the descent, which results not very natural in the iterative process. On the other hand, as the disequilibrium degree indicator that we propose here is bounded -in fact, normalized between 0 and 1-, it allows to treat each particle only in relation with its own potential equilibrium degree and independently of the relative distance to the rest of the particles.

In any case, the more substantial difference between our approach and classical methods is that the determination of the advance direction and the step size is completely independent of the parametrization that has been chosen for the surface $S$. Regarding to the direction, that independence has already been made clare. As for the step size some considerations must be made. Given an initial configuration, it must exist a unique stationary point for $\mathcal{I}$ such that the particles arrive to it following the direction $w_i = \dfrac{F_i^T}{|F_i|}$. Consequently, from the point of view of Mechanics, these directions not only can be understood as energy descent directions, but also as the velocity fields of the paths described by the particles in

its movement towards the equilibrium. This approach allows us to look at the optimization problem from the dynamic systems perspective. The step size will be chosen by applying an explicit forward Euler method to the system of ODE whose solutions are precisely these paths. These ODE are raised in a natural way in the coordinates of the ambient space and its numerical integration fixes a displacement for each particle in that space. In general, the application of that displacement takes the particles out of the surface $S$, which generates the need of considering an algorithm to return the particles to the surface in each iteration. Maybe the most versatile and simple one consists in using the gradient field of an implicit representation of the surface. In the examples that are included in the present paper - the sphere and the cube- that process results trivial. When the surface is described in a parametric form, the composition with the metric allow us to transfer to the parametric space the magnitude of the step to apply, which solves the return problem.

To make an exhaustive mechanical treatment of the problem is out of place, since it is not decisive with regards to the development of the algorithm. Nevertheless, we consider of interest to make some considerations from this point of view. If $x(t) = (x_1(t), \dots, x_N(t))$ denotes the position of $N$ particles in the instant $t$, then an equation for the movement of the system on a surface $S$ can be

$$x''(t) = -\nabla \mathcal{I}(x(t)) - cx'(t) + \Phi(x(t), x'(t)). \tag{2}$$

The term $-cx'(t)$, with $c > 0$, represents a dissipative force of viscous nature and $\Phi = (\Phi_1, \dots, \Phi_N)$ is an additional force that takes into account the interaction between each particle and $S$. For each $i = 1, \dots, N$, the normal component of $\Phi_i$, $\Phi_i^n = \rho\,|x_i'|^2 - F_i^n$, cancels the normal component of $F_i$ and provides the centripetal force, being $\rho$ the normal curvature in the direction of $x_i'$ at $x_i \in S$. The tangent component $\Phi_i^T$ considers the friction with $S$ and its expression depends on each particular model. If the friction force is not considered, then it is easy to prove that as $c \to \infty$ the trajectories that solve (2) tend to be the enveloping of the vectors $F_i^T$, see [3]. Hence, in this case the particles follow the direction of $-\nabla \mathcal{I}_{|M}$. It is possible to propose a friction model such that the corresponding trajectories tend to be the enveloping of the vectors $w_i$.

Therefore, the search for the minimum of the energy will be carried out obtaining the paths described by the particles in its movement towards the equilibrium. These ideas belong to the fundamentals of Rational Mechanics and have already been used in the literature by different authors, see for example [9, 12, 15]. However, in many cases the equilibrium of the particles is purely heuristic and it does not come from the minimization of an explicit functional, and, anyway, the objective is not to localize the equilibrium configuration as a goal in itself, but to arrive to a reasonable level of approximation.

In short, the system of ODE to solve is

$$x' = w. \tag{3}$$

For its numerical resolution we will use the following explicit forward Euler method:

$$x^{k+1} = x^k + a\,\varphi(x^k)\,w^k \tag{4}$$

where $a$ is a positive scalar that depends on the kernel and on the surface $S$, and $\varphi(x^k)$ depends on the current position of all the particles of the system and allows us to adapt the step size to the difficulty of the different configurations that appear during the calculation. The step size must be reduced when there exist very close particles in order that they do not "run helter-skelter" breaking the continuity of the movement, whereas if the relative distances grow, the step size can be increased in benefit of the convergence ratio. An appropriate choice is

$$\varphi(x) = \min_{1 \le p < q \le N} \{|x_p - x_q|\},$$

according to which $a\,|w_i|$ represents the fraction of the minimum distance between particles that the $i$-th one advances in each iteration.

The numerical experimentation carried out until now confirms that our algorithm converges -in the sense that it localizes an equilibrium position- even for crazy initial positions, for instance the corresponding to confine the $N$ particles in the $N$-th part of the area of the surface. However, in general, the algorithm is not stable, in the sense that for each initial position it does not necessarily localize the unique equilibrium position corresponding to it. An stable algorithm would require an excessive computational cost due to the existence of a great quantity of stationary points extraordinarily close, although in any way this type of stability is not really important since the convergence is guaranteed.

# 3 The Unit Sphere

The problem of obtaining Fekete points in the unit sphere is probably the most characteristic both for its hardness and for its different applications. From a numerical point of view we can mention the Ph.D. of Y. Zhou [16] and some works generated around it [10], [11]. In that Ph.D. minimum energy configurations are presented for each $N \le 200$ for the Newtonian and logarithmic kernels and for the kernel of the distance. The algorithms used were quasi-Newton after the elimination of the constraints by means of the stereographic projection. In view of these results and other ones of theoretical character, extrapolation formulae for the minimum energy associated to those kernels in the sphere were proposed. Recently, some works have appeared in which good configurations of 1600 points obtained by means of $ad - hoc$ algorithms are presented, see [4].

In the unit sphere, after the generation of an arbitrary initial configuration $x^0$ of $N$ different points, the $k$-th iteration of our algorithm simply consists in:

-Calculate the advance direction $w^{k-1}$.

-Calculate $\hat{x}^k = x^{k-1} + a\,d_{k-1}\,w^{k-1}$.

-Obtain the $k$-th configuration: $x_i^k = \dfrac{\hat{x}_i^k}{|\hat{x}_i^k|}$.

The minimum distance $d_{k-1}$ between two points of the $(k-1)$-th configuration is obtained

| **Kernel** | Distance | Logarithmic | Newtonian | Riesz $s = 2$ | Riesz $s = 3$ |
|---|---|---|---|---|---|
| $\boldsymbol{a}$ | 10 | 8 | 1 | 0.1 | 0.02 |

Table 1: Reference values for the coefficient $a$

as a byproduct of the advance direction calculation. It is necessary to indicate that, for the kernels we are interested in, the most expensive step of the iterative process is precisely the calculation of this direction, that involves $N^2$ operations. In Table 1 we show reference values for the coefficient $a$ for some kernels.

To study the convergence of our algorithm, we use $\max_{1\leq i\leq N} |w_i|$, *i.e.*, the maximum disequilibrium degree of the particles, as a measure of the error. If we analyze the evolution of the error with respect to the iteration number, we observe that a linear convergence ratio is systematically attained after a first highly non-linear stage. When the linear stage is reached the particles can be supposed to be sufficiently close to a stationary point, in the sense that from this moment the Newton algorithm can be used with guaranty of convergence. Figure 2 (a) illustrates the behavior of the error for a configuration of 1000 particles with the Newtonian kernel.

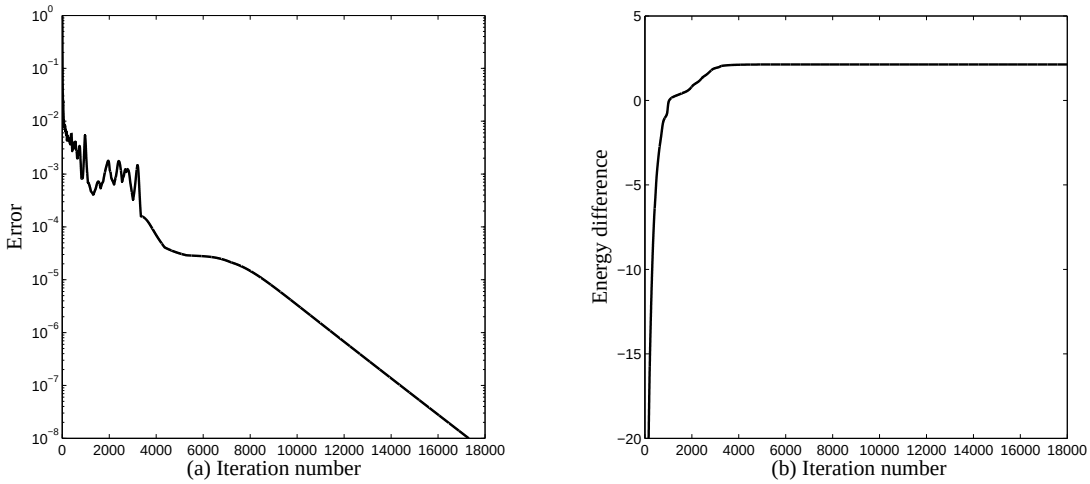


Figure 2: The behavior of the algorithm

Figure 2 (b) displays the evolution of the difference between the energy corresponding to the extrapolation formula given in [16] and the energy computed by our algorithm. We must note that the energy given by the formula, in spite of been accurate, can be improved very quickly. In fact, this happens long before the linear tendency is reached. Figure 3 shows the initial and final configurations of the non-linear stage for the previous case as well as the Dirichlet cells of both configurations. The initial configuration was generated randomly adjusting the distribution of the particles to a uniform probability density on the sphere. We must note that the energy produced by the initial configuration is 500144.450659, and

after the iterative process the energy value is 482534.789049, which represents only a 3.5% of decrease. On the other hand, the algorithm shows a high efficiency, since the time required to reach the linear tendency was around 15 minutes and to surpass the extrapolated energy value required only around 2 minutes.

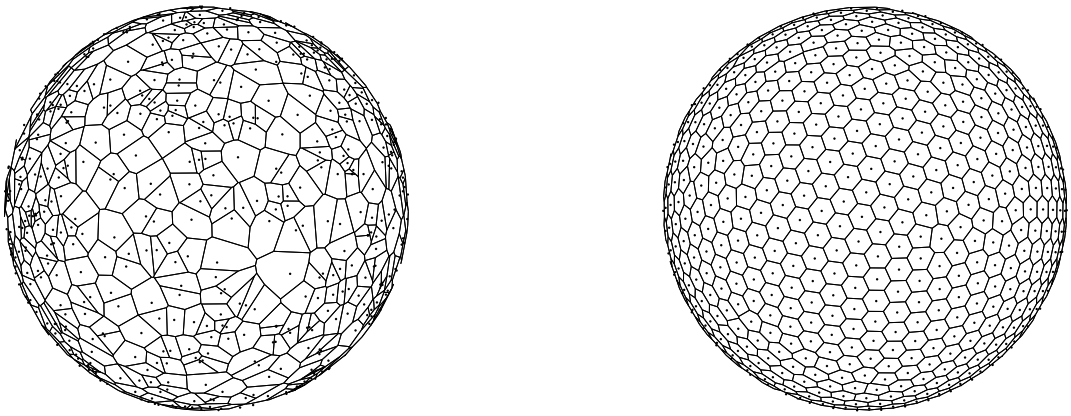

Figure 3: 1000 particles and their Dirichlet cells for the iterations 0 and 8000

Figure 4 shows a configuration of 5000 particles when the linear tendency has been attained, which required approximately 20 hours of calculation time. With a configuration of 50000 particles, working also with the Newtonian kernel and without considering any kind of symmetry, the time required to improve the energy corresponding to the extrapolation formula has been of approximately 15 hours.

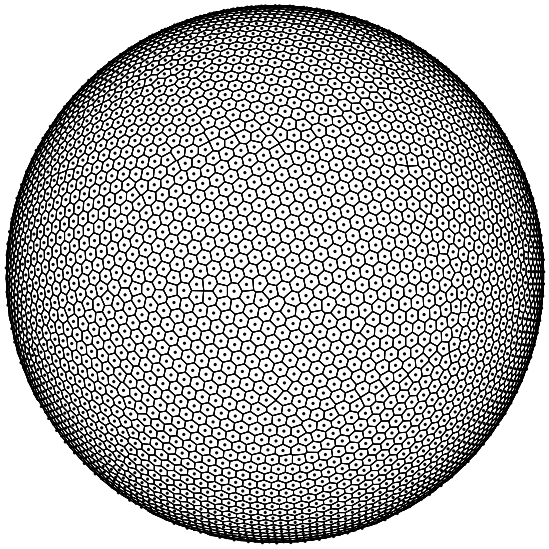

Figure 4: A beautiful configuration and the Dirichlet cells for $N = 5000$

The numerical experimentation carried out until now is not enough to extract definitive conclusions about the total cost needed to obtain a near-equilibrium configuration. Never-

theless, the results obtained allow us to be optimistic in that sense, and they seem to suggest an average computational cost of order less than $N^3$. It must be considered that in such a non-linear problem, some fluctuations in the cost are natural. For instance, for fixed $N$ similar initial configurations could require different calculation times, whereas configurations with more particles than others could require less iterations. It is clear that the memory requirements are of order $N$. Moreover, the tests realized until now confirm the robustness of the algorithm, see [3].

To obtain good equilibrium configurations for a great number of particles without an increase in the calculus infrastructure, we can use the symmetries of the sphere. Good initial configurations that take into account symmetries are the geodesic grids. In particular, we consider families of truncated icosahedron, which correspond to use 120 symmetries. Although the geodesics constitute an excellent family of initial configuration, they do not present an uniform density of points. This is due to the projection that takes the points from the faces of the icosahedron to the sphere. In this conditions our algorithm basically smooths the density, as can be seen in Figure 5. In it we represent the initial and final positions of the points corresponding to a face of the original icosahedron for a configuration with 12002 particles in total.

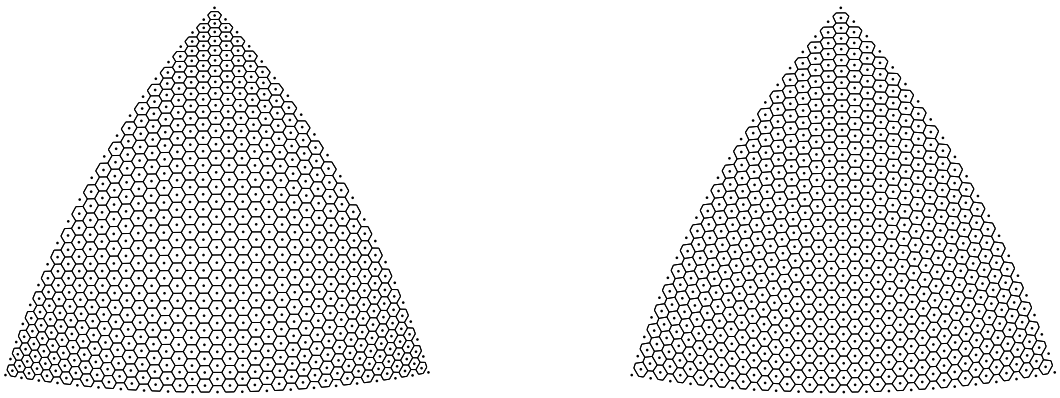

Figure 5: Initial and final configurations in a spherical triangle

In Figure 6 we present the convergence evolution for several configurations whose initial positions are defined by different frequency geodesic grids when the Newtonian kernel is considered. The total number of particles for each one of the seven cases considered are: (1) $N = 4322$, (2) $N = 12002$, (3) $N = 27002$, (4) $N = 52922$, (5) $N = 100922$, (6) $N = 201722$, (7) $N = 300002$. Note that the evolution of the error is very smooth even before the final linear tendency is attained. A reason for that is the great quality of the initial configurations. Moreover, it must be observed that all geodesics of this family start with approximately the same error. This fact can be used to realize an analysis of the cost in similar conditions. If we consider the reference error $\mathsf{e} = 5 \cdot 10^{-3}$, we can obtain in each case the number of iterations needed to attain $\mathsf{e}$. This is showed in Figure 6 as well as a simple interpolation of the data.

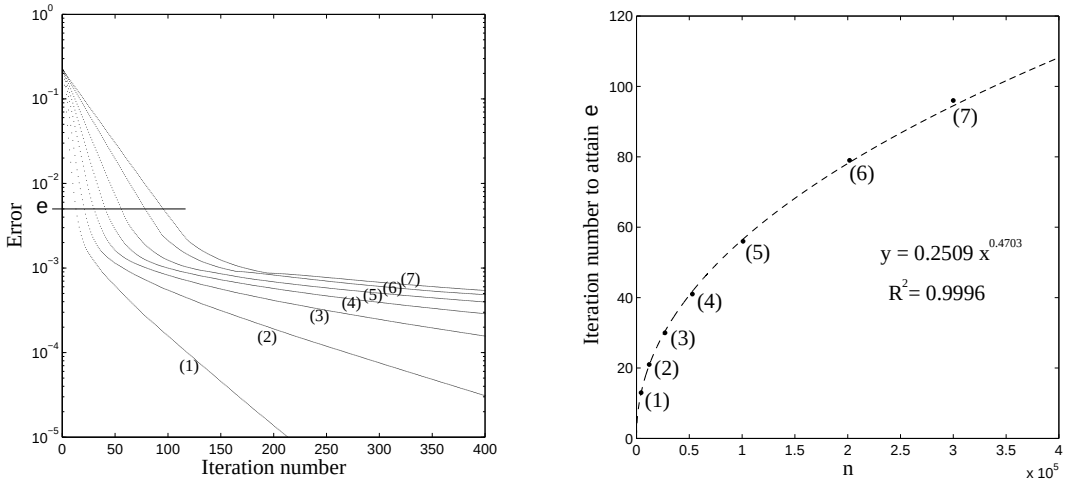


Figure 6: The behavior of the algorithm with geodesics

# 4 The Unit Cube

We aim here at presenting some results obtained by applying our algorithm in the unit cube. In this way the versatility of the method will be showed clear since the cube has a geometry radically different to the sphere one. It is evident that the unit cube does not verify the regularity properties required to dispose of a normal vector in each point. Nevertheless, we have considered its 48 symmetries reducing the domain to a triangle representing the eighth part of the cube face. In this case, the Newtonian kernel is especially interesting, since its corresponding Fekete points tend to reproduce the electric charge density in electrostatic equilibrium on the cube, which is itself a classical question.

An important accumulation of particles near the edges of the cube would occur, since the density presents asymptotes in them and hence the difficulty when searching for Fekete points increases. However, we want to emphasize that the behavior of the algorithm in the cube is essentially the same than in the sphere and this is fundamentally due to the choice of $w$ as advance direction. Other possible choices, as for example $\breve{w}_i = \dfrac{F_i^T}{|F_i|_{max}}$, which is equivalent to follow the gradient direction, clearly leads to unsatisfactory results.

Figure 7 shows a near-equilibrium distribution in a face of the cube for a total quantity of 47520 particles, which corresponds to 990 particles inside of the reference triangle. The same figure shows the convergence of the method. The linear tendency is approximately reached at iteration 40000.

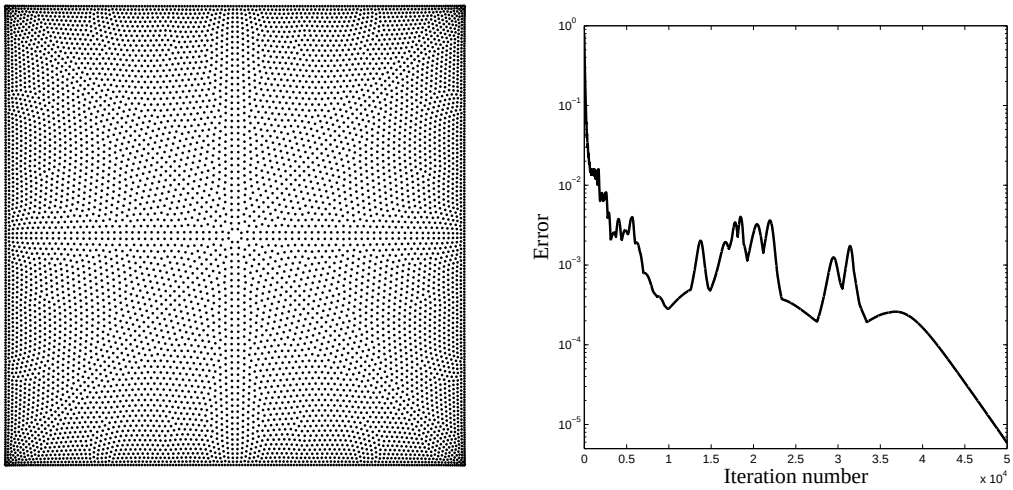


Figure 7: 7920 particles in a cube face and the convergence of the method

## Acknowledgements

The authors express their sincere gratitude to Professor Antonio Gens by his unconditional support. This work has been partially supported by the CICYT under project BFM2003-06014.

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