Point Distribution on Bidimensional Sphere

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Outline

1. The Fekete problem and Smale's 7th problem.
2. The Forces method.
3. The FinisTerrae challenge.

1.1 The Fekete problem

We call *the Fekete problem* that of determining the N-tuples of points $\omega_N = \{x_1, \ldots, x_N\},\ x_i \in \mathbb{R}^d$, that minimize on a compact set $S \subset \mathbb{R}^d$ a potential energy functional $\mathcal{I}_N$ that depends on the relative distances between the *N* points. The N-tuples ω_N are called *the Fekete points*.

Logarithmic energy:

$$\mathcal{I}_N(x) = \sum_{1 \le i < j \le N} \log \frac{1}{|x_i - x_j|}$$

Riesz's energies:

$$\mathcal{I}_N(x) = \sum_{1 \le i < j \le N} \frac{1}{|x_i - x_j|^s}$$

General case: $s > 0$

Newtonian energy: $s = d - 2$

Best-packing problem: $s \longrightarrow \infty$

Applications: Physics, Numerical Methods, Complexity Theory.

1.2 Smale's 7th problem

¿It is possible to design an algorithm that finds a configuration x of points on the 2-sphere satisfying the condition

$$\mathcal{I}_N(x) - \mathcal{I}_N(\omega_N) \leq c \log N$$

in time polynomial in N ?

Here $\mathcal{I}_N$ represents the logarithmic potential energy and ω_N are the Fekete points associated with this energy on the 2-sphere.

It is known that

$$\mathcal{I}_N(\omega_N) = -\frac{1}{4} \log\left(\frac{4}{e}\right) N^2 - \frac{1}{4} N \log N + O(N)$$

2.1 The Forces method

$$x = \{x_1, \dots, x_N\},\; x_i \in S \subset \mathbb{R}^3$$

$$-\nabla \mathcal{I}_N = (F_1, \dots, F_N)$$

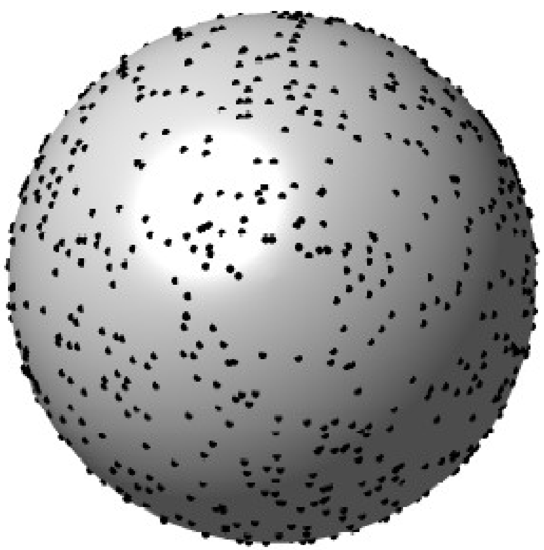
$$-\nabla \mathcal{I}_N|_{S^N} = (F_1^T, \dots, F_N^T)$$

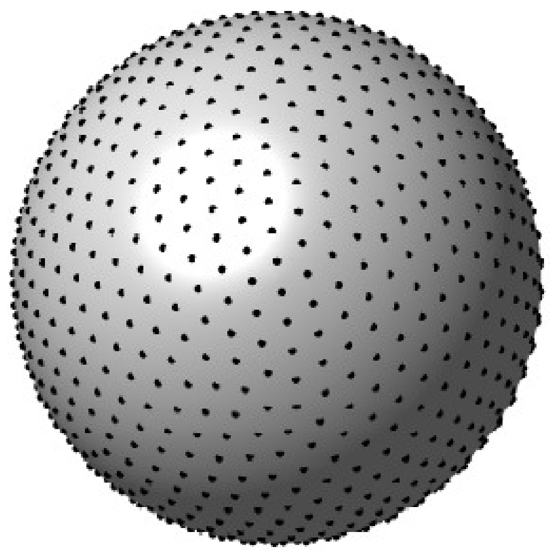
$$\boxed{x^{k+1} = x^k + a \min_{1 \le i < j \le N} \{|x_i - x_j|\}\, w^k}$$

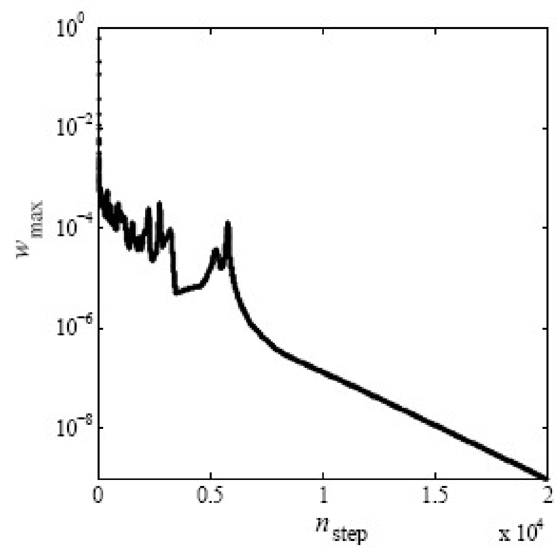
+ return algorithm

$$w = (w_1, \dots, w_N) \qquad w_i = \frac{F_i^T}{|F_i|}$$

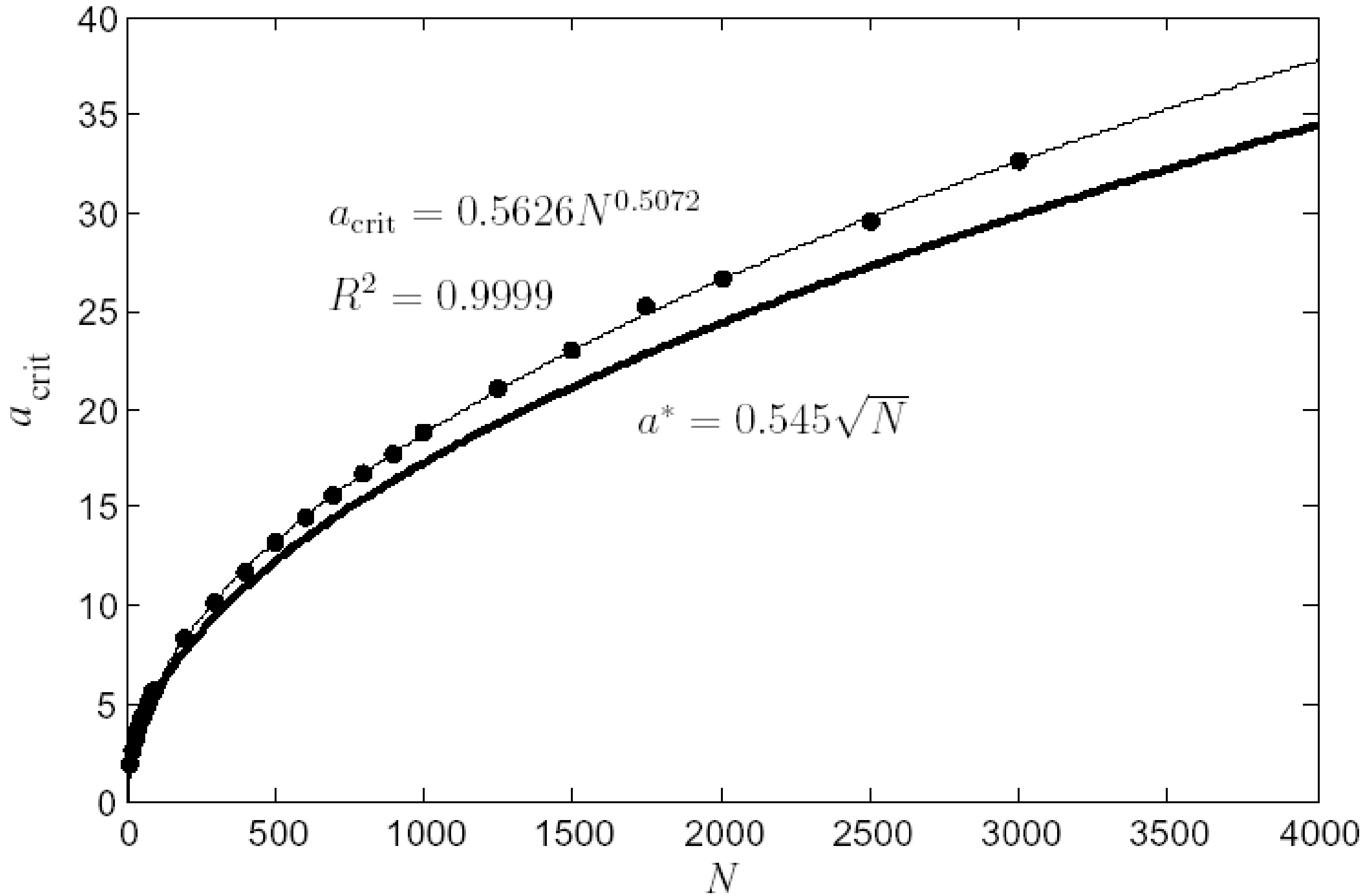
$$w_{\max} = \max_{1 \le i \le N} |w_i|$$





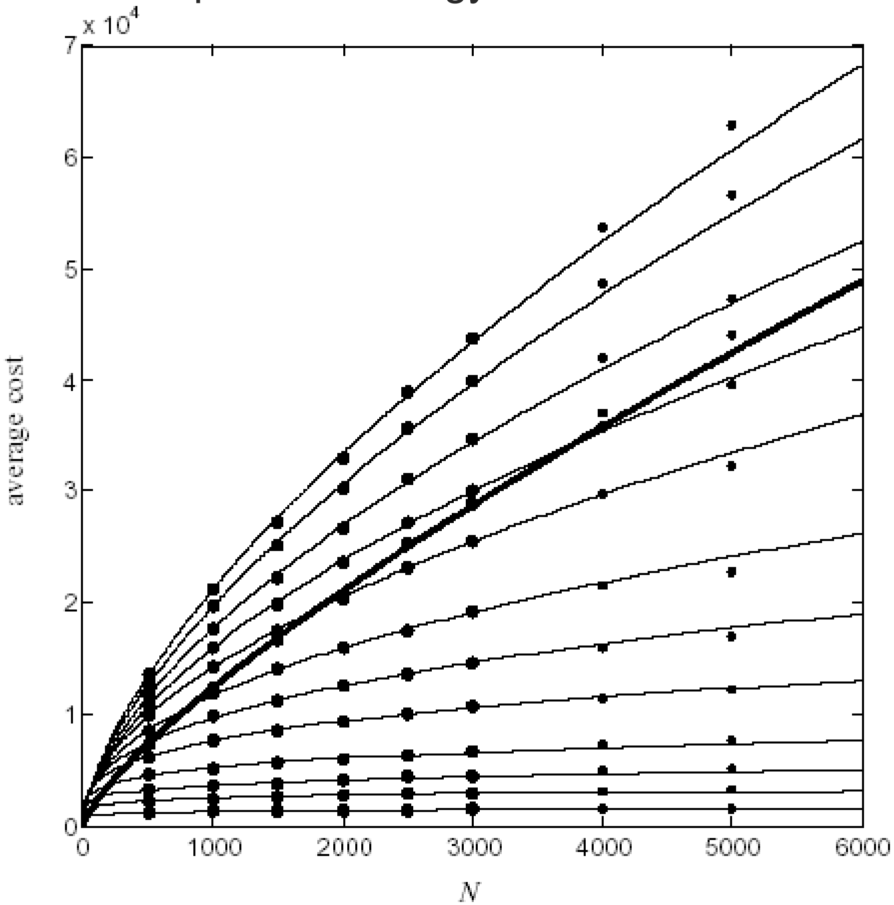


2.2 The coefficient *a*



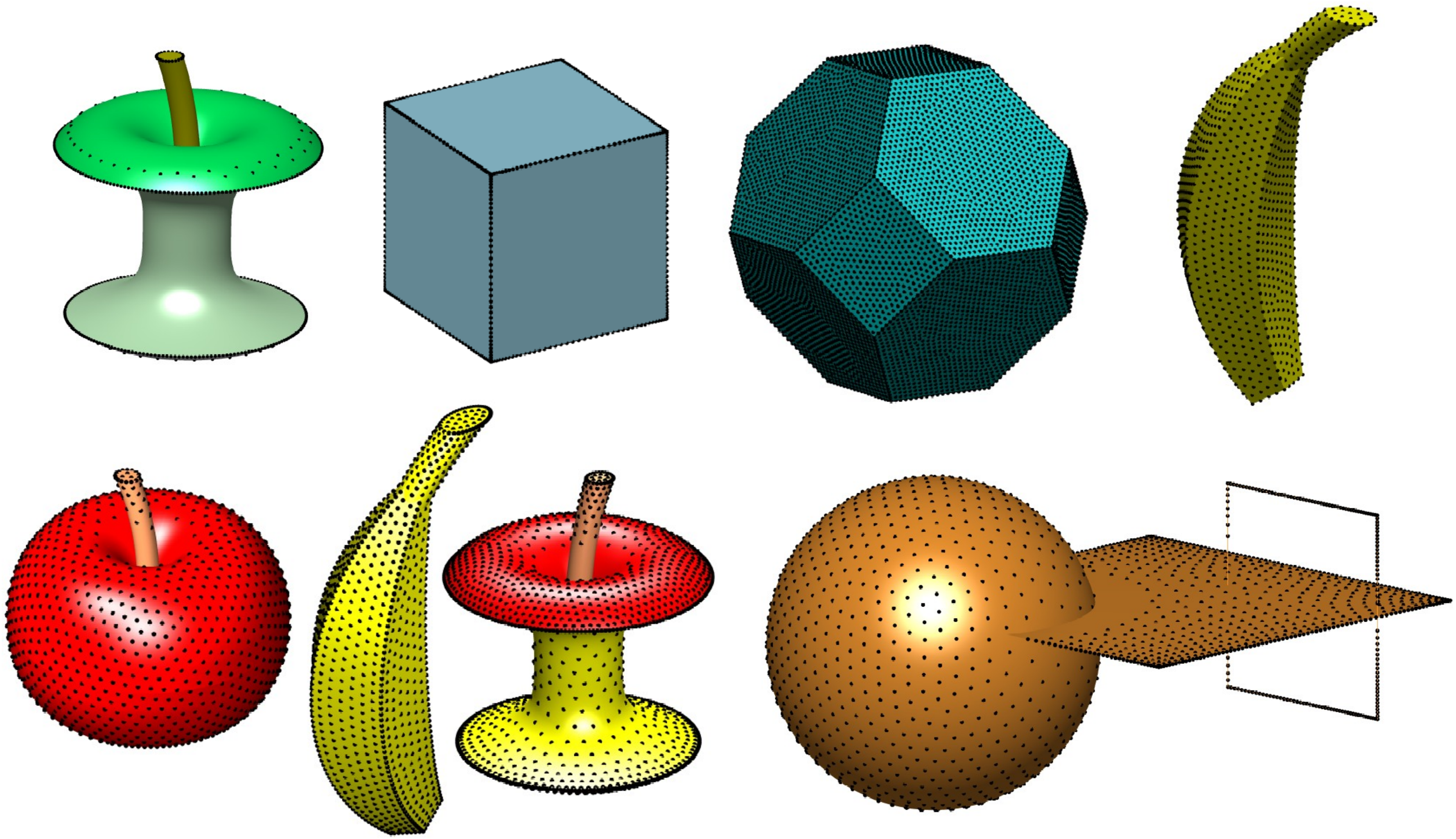
2.3 The cost of a local minimum

Cost at each step: the logarithmic energy requires only elementary operations for the actualization of the forces (O(N^2) operations), since it is not necessary to compute the energy.



ε	γ	p	R^2	$N_\perp$
$5 \cdot 10^{-5}$	543.64	0.1161	0.9892	28
$2 \cdot 10^{-5}$	818.92	0.1521	0.966	67
$1 \cdot 10^{-5}$	1043.4	0.1774	0.9732	121
$5 \cdot 10^{-6}$	1119.0	0.2197	0.9936	200
$2 \cdot 10^{-6}$	932.67	0.3026	0.9979	347
$1 \cdot 10^{-6}$	684.91	0.3819	0.9987	520
$5 \cdot 10^{-7}$	505.6	0.4536	0.9992	824
$2 \cdot 10^{-7}$	351.02	0.5349	0.9997	1794
$1 \cdot 10^{-7}$	297.33	0.5761	0.9996	3776
$5 \cdot 10^{-8}$	264.28	0.608	0.9996	9353
$2 \cdot 10^{-8}$	240.28	0.6376	0.9994	35989
$1 \cdot 10^{-8}$	229.7	0.6546	0.9994	116855
nr	61.306	0.7678	0.9995	

2.4 The versatility of the method



3.1 The FinisTerrae challenge

3.2 The FinisTerrae challenge

Large scale experiments:

I. The cost of a local minimum (150000 hours):

-For N=10000, a total of 1000 runs attaining an error of 10^{-9} .
-For N=20000, a total of 100 runs attaining an error of $5 \cdot 10^{-10}$.
-For N=50000, a total of 10 runs attaining an error of 10^{-10} .

II. Robustness (40000 hours, 1024 CPUs working in parallel):

-For $N=10^6$, a total of 3000 steps from a delta starting position.

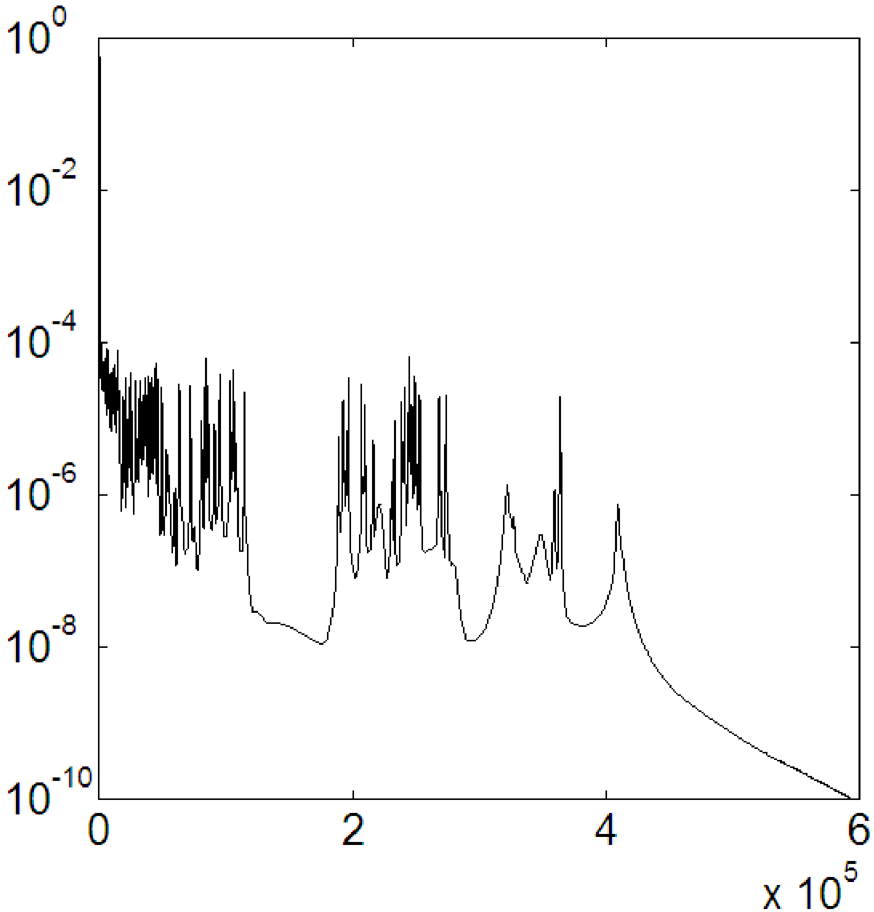
III. Sample information for Smale’s 7th problem (160000 hours):

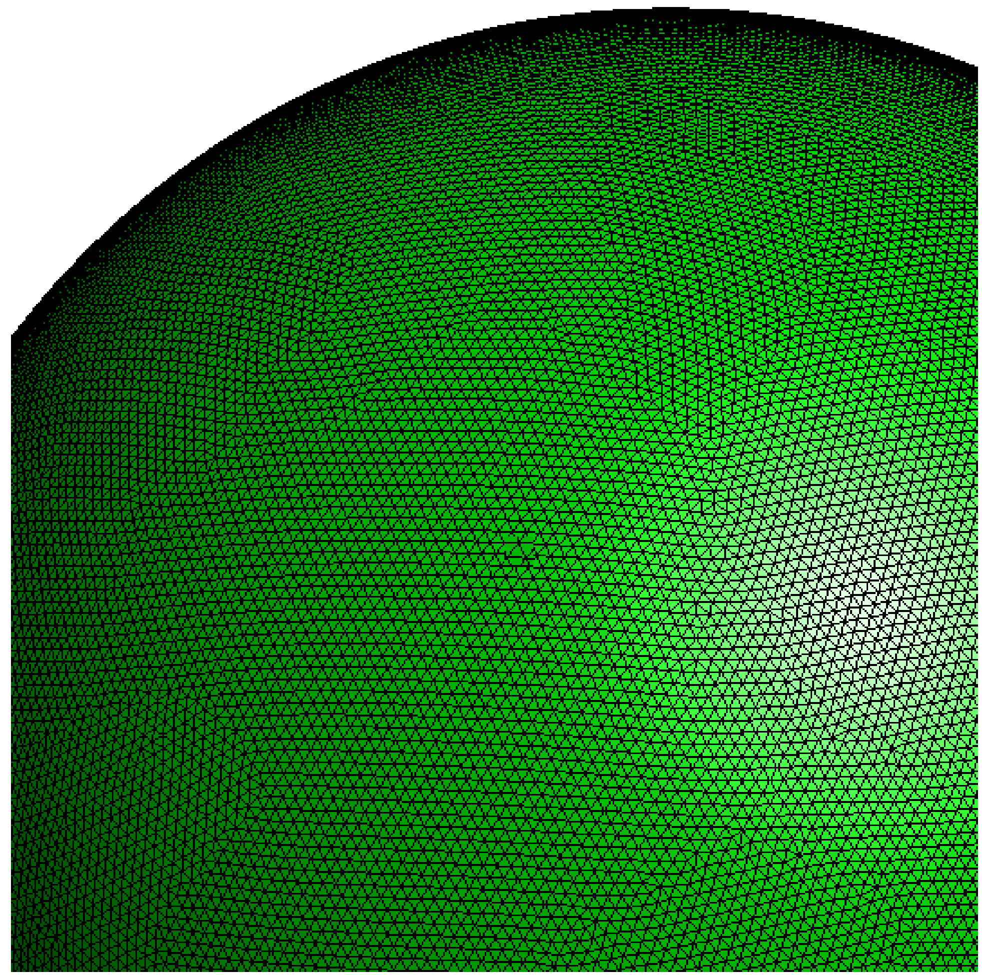
-Almost $5.1 \cdot 10^7$ runs for different *N* between 300 and 1000.

3.3 The FinisTerrae challenge

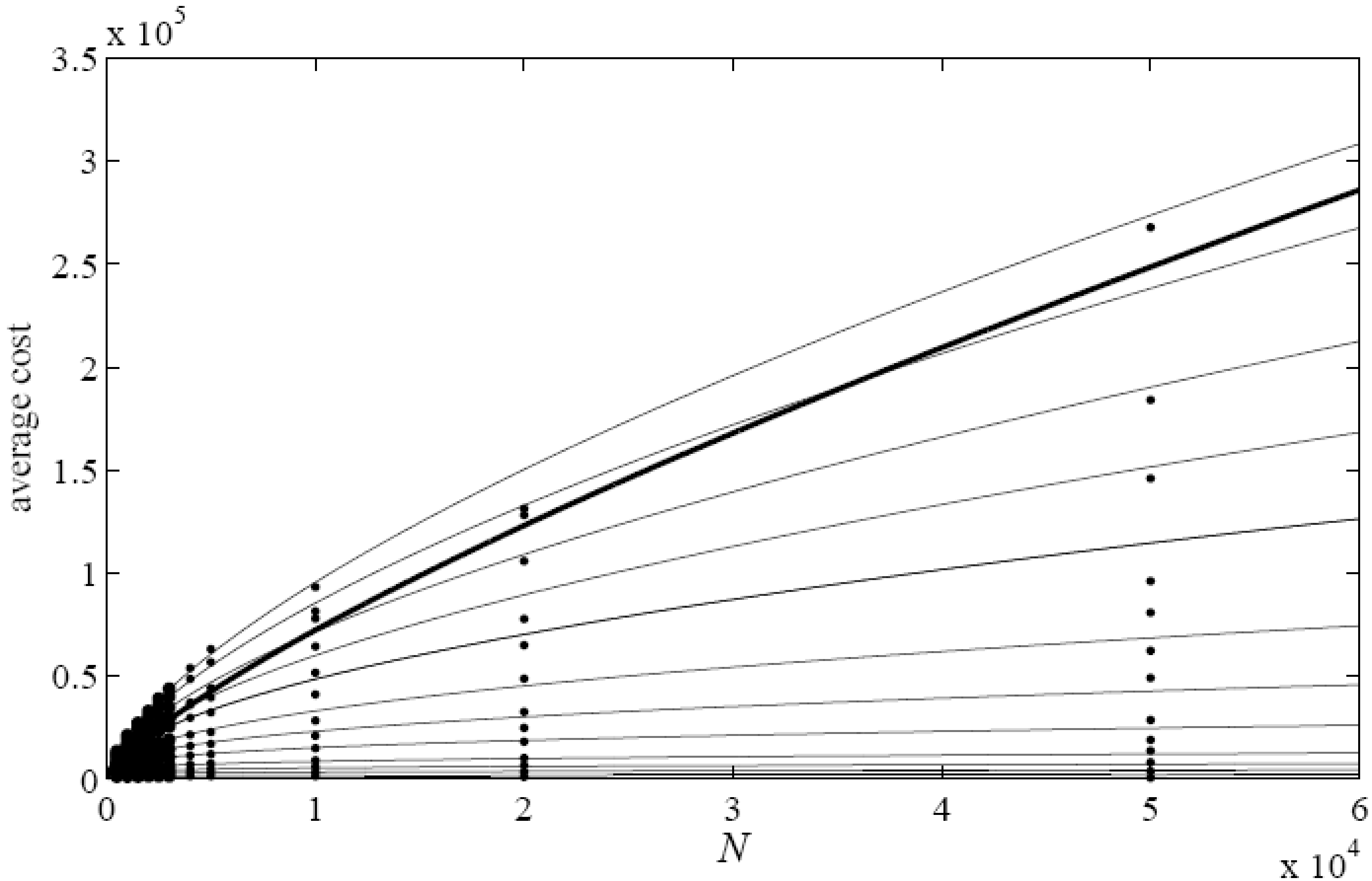
N	Clonetroop					FinisTerrae						Total
	$\varepsilon=5\cdot10^{-7}$	$\varepsilon=2\cdot10^{-7}$	$\varepsilon=10^{-8}$	$\varepsilon=10^{-10}$	Subtotal	$\varepsilon=5\cdot10^{-7}$	$\varepsilon=2\cdot10^{-7}$	$\varepsilon=10^{-9}$	$\varepsilon=5\cdot10^{-10}$	$\varepsilon=10^{-10}$	Subtotal	
87					120000*							120000
200					60000*							60000
300	2723100	100100			2823200	4800000					4800000	7623200
400	1125864	100100			1225964	3858995					3858995	5084959
500		974410	5005	100000	1079415	28155617	1705627				29861244	30940659
600	900015	100100			1000115		9836186				9836186	10836301
700		1000115			1000115		407298				407298	1407413
800		1000115		100000	1100115		380387				380387	1480502
900		100100			100100		442822				442822	542922
1000		100100	5010		105110		1138201				1138201	1243311
1500			7005		7005							7005
2000			5474		5474							5474
2500			5333		5333							5333
3000			5474		5474							5474
4000			1479		1479							1479
5000			1183		1183							1183
10000								1000			1000	1000
20000									100		100	100
50000										10	10	10
1000000											1*	1
	Total Clonetroop				**8640082**	**Total FinisTerrae**					**50726244**	
Total data												**59366326**

3.4 The FinisTerrae challenge I



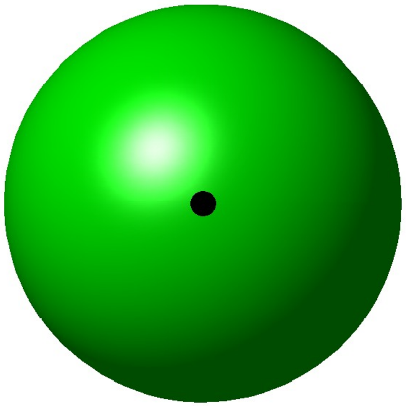


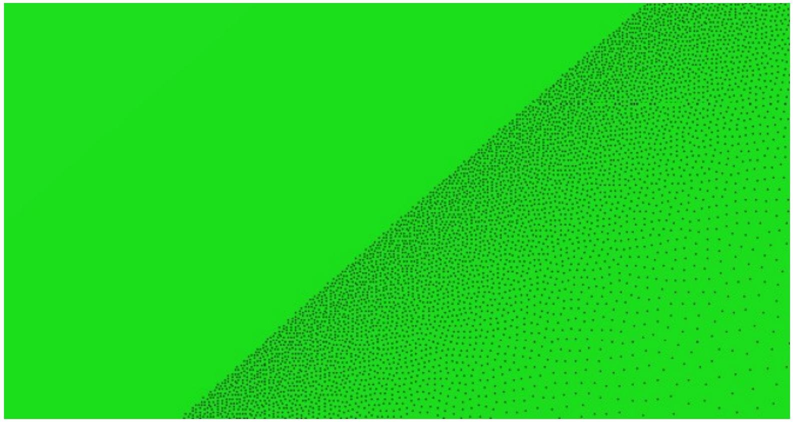
3.5 The FinisTerrae challenge I

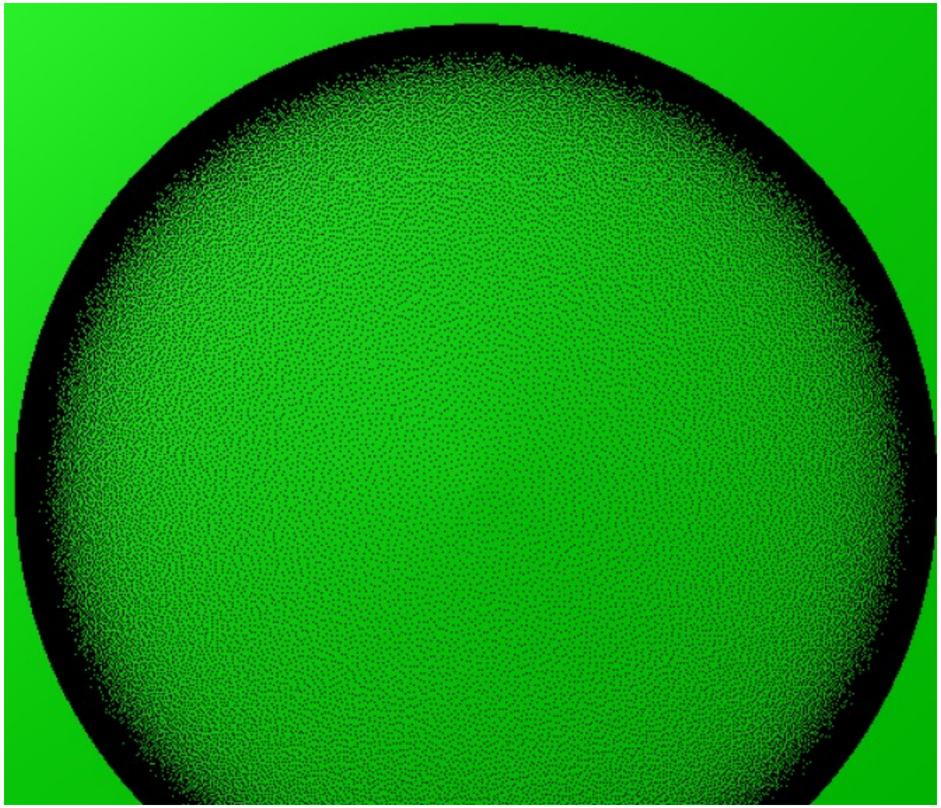


3.6 The FinisTerrae challenge II

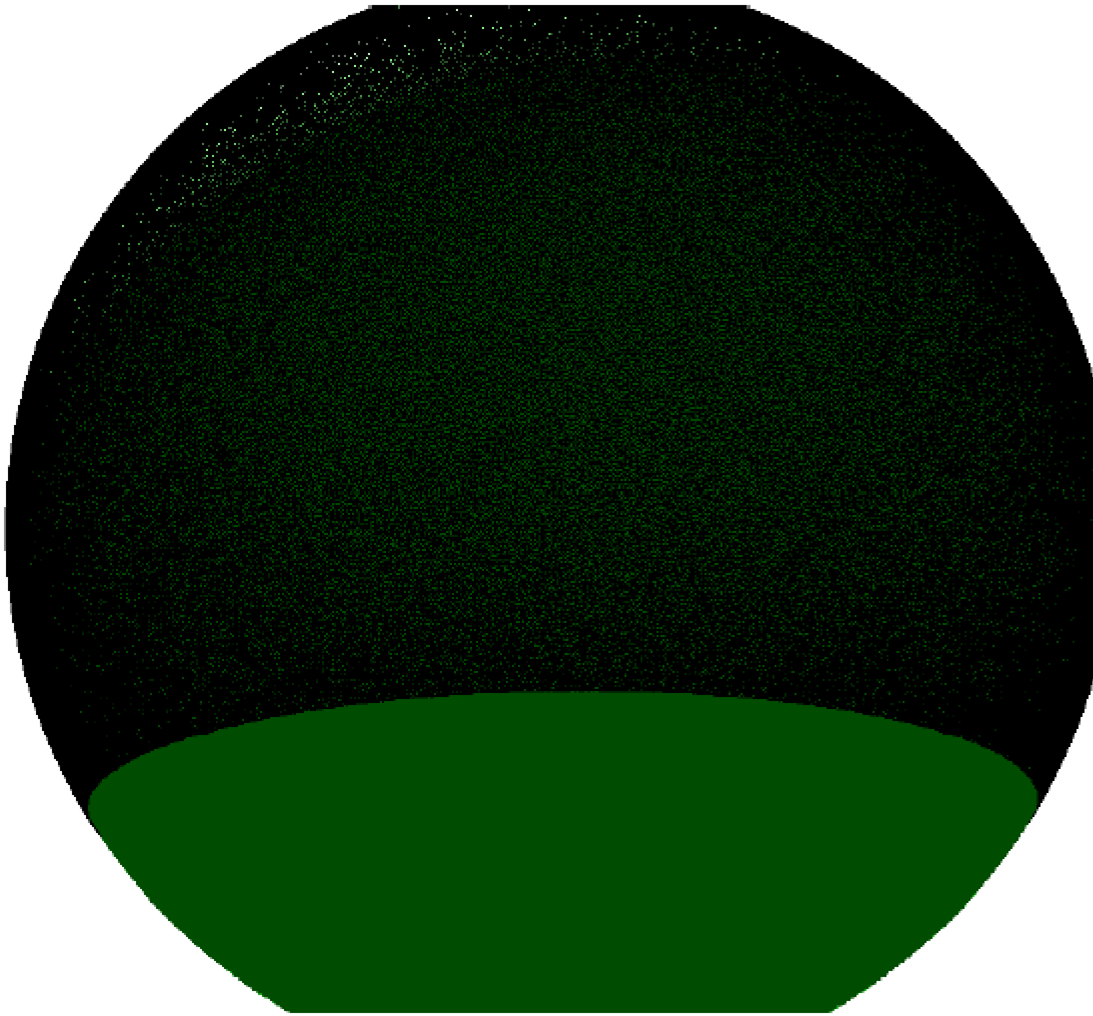
$$a = a^* = 0.545\sqrt{10^6} = 545$$



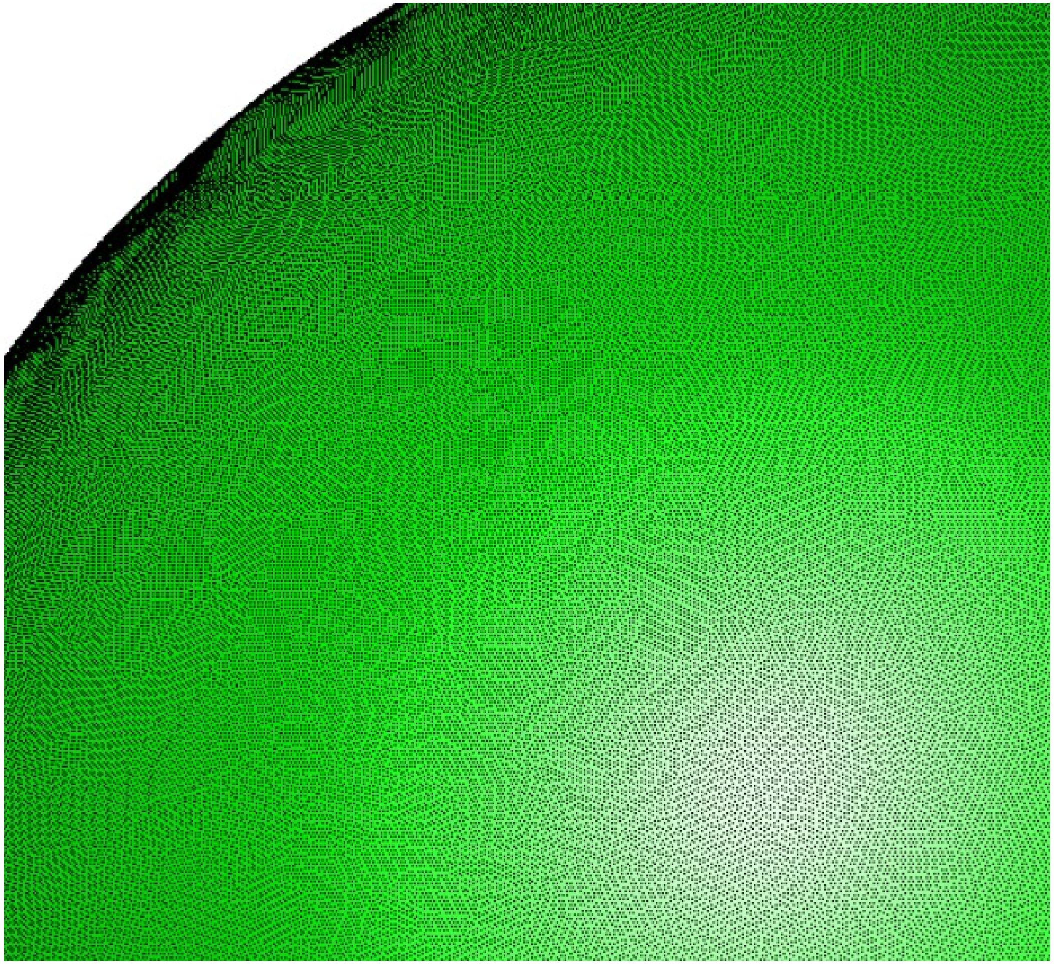


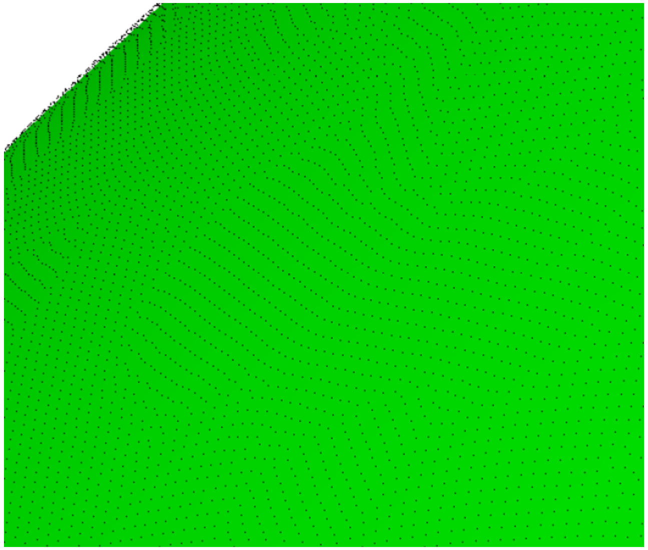


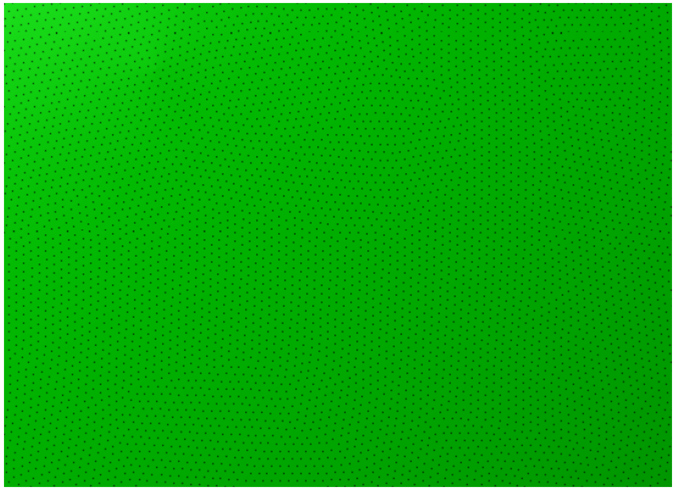
3.7 The FinisTerrae challenge II



3.8 The FinisTerrae challenge II







3.9 The FinisTerrae challenge III

Smale's 7th problem:

$$\mathcal{I}_N(x) - \mathcal{I}_N(\omega_N) \leq c \log N$$

Key questions:

-~~¿Which is the cost of a local minimum?~~

-¿Which is the value of $\mathcal{I}_N(\omega_N)$?

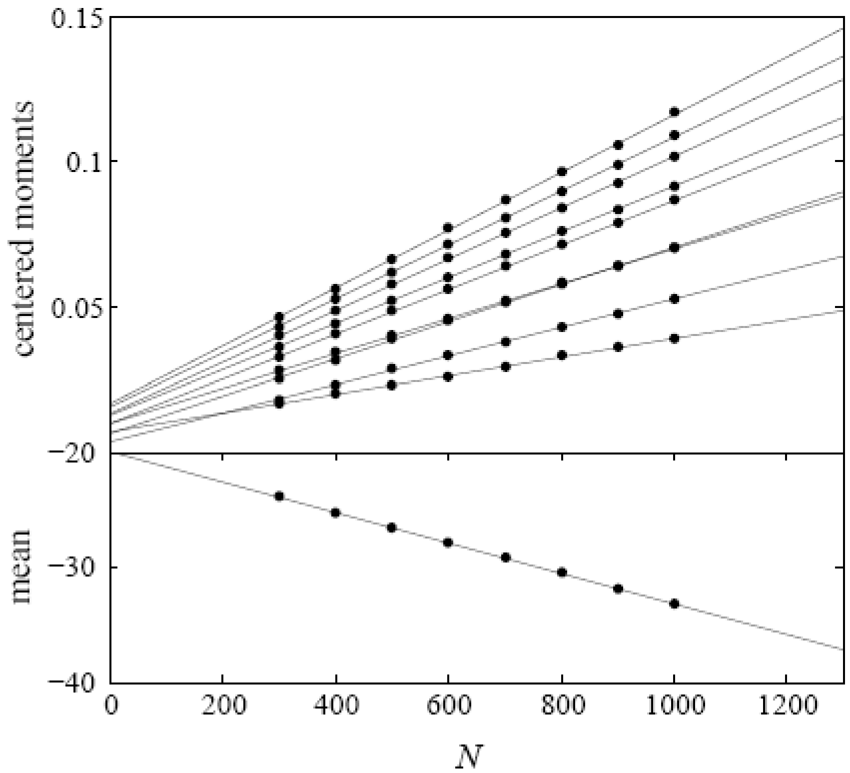
$$\mathcal{I}_N(\omega_N) = -\frac{1}{4}\log\left(\frac{4}{e}\right)N^2 - \frac{1}{4}N\log N + O(N)$$

-¿Which is the probability of finding a minimum satisfying Smale's conditions?

3.10 The FinisTerrae challenge III

$$U = I + \frac{1}{4}\log\left(\frac{4}{e}\right)N^2 + \frac{1}{4}N\log N \qquad V = \frac{U-\mu_U}{\sigma_U}$$

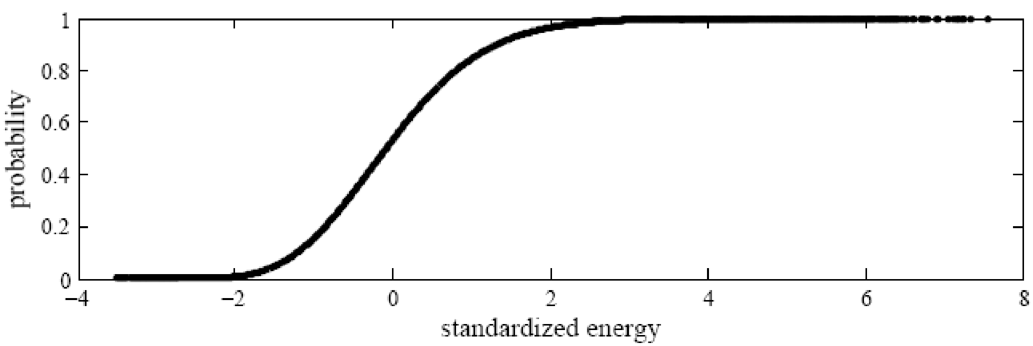
$$\mu_U \simeq A_1 N + B_1 \qquad (M_U^k)' \simeq (A_k N + B_k)^k \qquad M_V^k \simeq \left(\frac{A_k N + B_k}{A_2 N + B_2}\right)^k$$

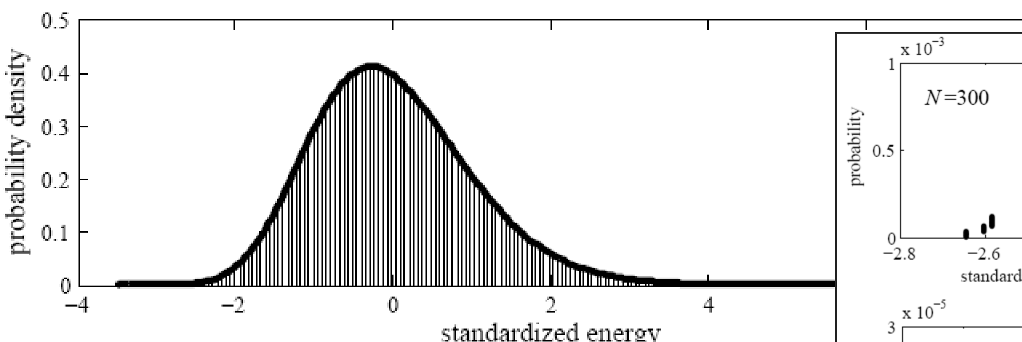


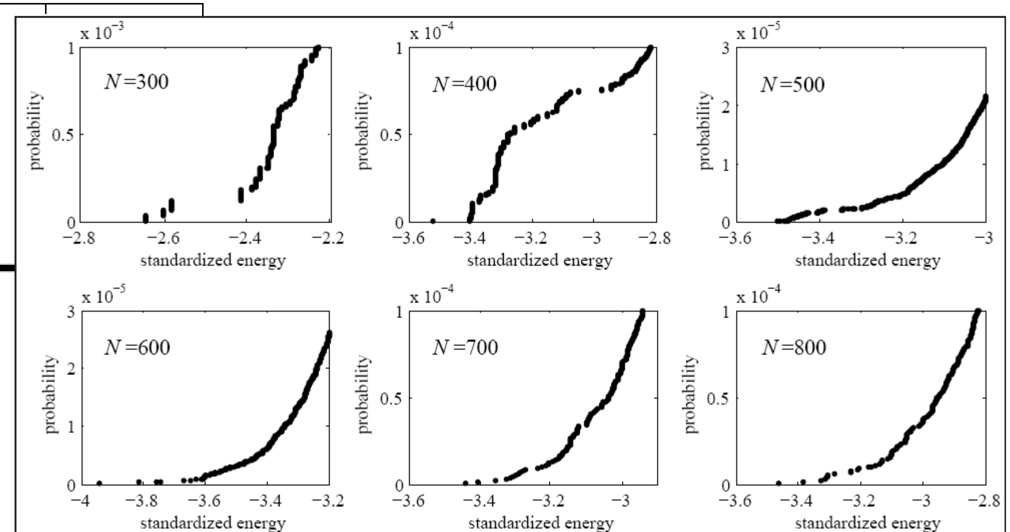
order	A_k	B_k	R^2
1	-0.026656	0.26882	0.99999
2	$4{,}9108 \cdot 10^{-5}$	0.0037473	0.99919
3	$3.2173 \cdot 10^{-5}$	0.0070638	0.99844
4	$6.4080 \cdot 10^{-5}$	0.0065284	0.99959
5	$6.0160 \cdot 10^{-5}$	0.010139	0.99987
6	$7.6660 \cdot 10^{-5}$	0.010067	0.99986
7	$7.8828 \cdot 10^{-5}$	0.012782	0.99996
8	$8.8477 \cdot 10^{-5}$	0.013589	0.99989
9	$9.2906 \cdot 10^{-5}$	0.015607	0.999854
10	$9.9627 \cdot 10^{-5}$	0.016875	0.999734

3.11 The FinisTerrae challenge III

Sample probability distributions:







3.12 The FinisTerrae challenge III

The theoretical model:

$$f_Z(x) = A^{-1} q_1(x) q_2(1-x)$$

$$W = \frac{Z - \mu_Z}{\sigma_Z}$$

$$h(x) = \frac{\log x}{x}$$

$$q_1(x, p, K_1) = \frac{1}{\left(K_1 x h^{-1}(K_1 x) - 1\right)\left(h^{-1}(K_1 x)\right)^{(p-1)}}$$

$$q_1(x, p, q, K_1) = \frac{\left(h^{-1}(K_1 x)\right)^{(q+1)}}{(K_1 x h^{-1}(K_1 x) - 1) e^{p(h^{-1}(K_1 x))^q}}$$

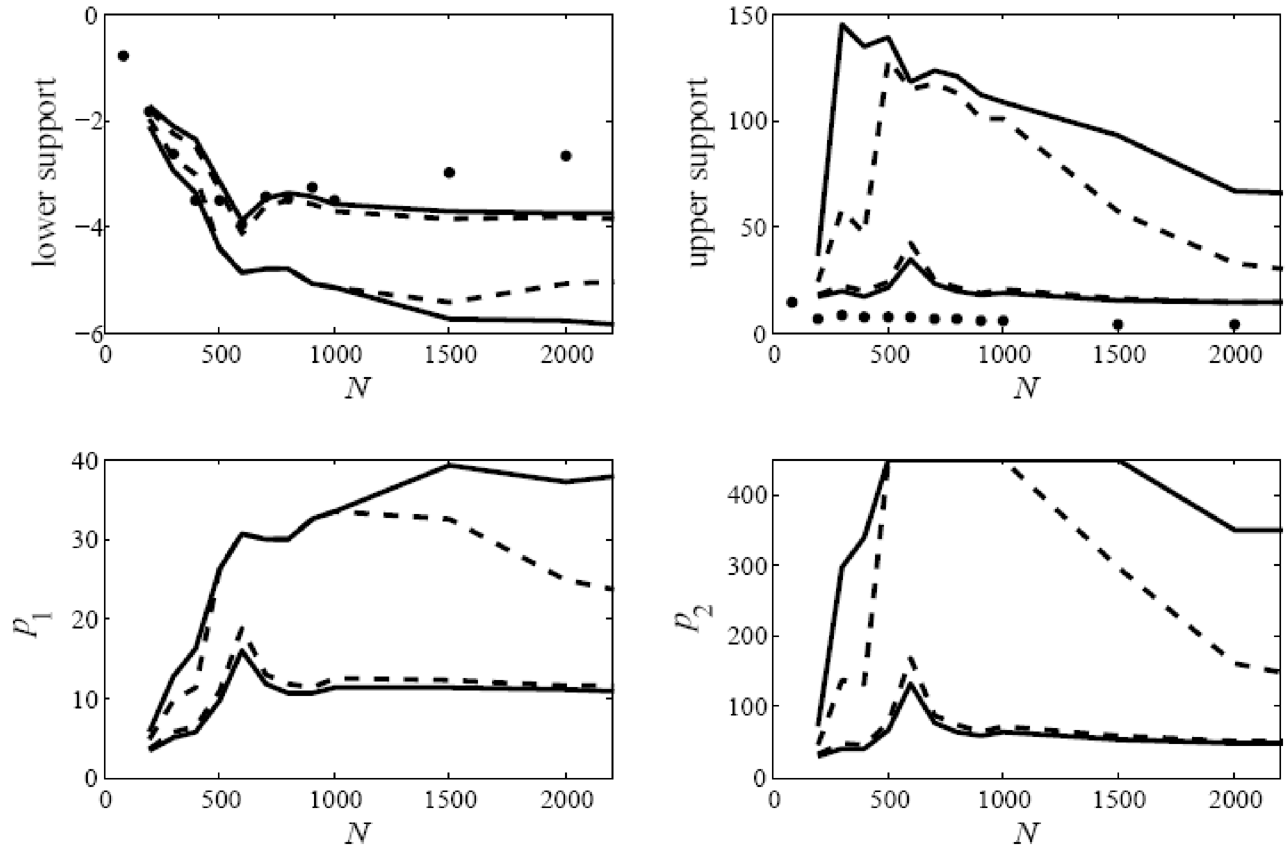
3.13 The FinisTerrae challenge III

A plausible probabilistic solution: the moments.

N	p_1	p_2	α_N	Ω_N	relative difference with the standardized sample moments							
					3	4	5	6	7	8	9	10
200	3.977	35.321	-1.856	19.642	0.002	0.008	0.000	0.009	-0.001	0.002	-0.005	-0.006
	4.426	41.563	-1.941	22.217	-0.005	0.007	-0.004	0.008	-0.002	0.003	-0.004	-0.004
300	8.927	113.798	-2.647	47.402	-0.009	-0.004	0.000	0.001	0.005	0.008	0.011	0.014
	6.064	54.940	-2.307	24.622	0.005	-0.005	0.001	-0.003	-0.001	-0.003	-0.002	-0.003
400	16.068	337.635	-3.368	134.785	-0.010	0.005	0.007	0.013	0.020	0.025	0.033	0.040
	11.239	130.741	-3.025	46.598	-0.009	0.001	0.002	0.005	0.008	0.011	0.016	0.019
500	26.247	450.000	-4.413	125.113	-0.009	0.001	0.000	0.004	0.006	0.008	0.011	0.013
	20.746	247.565	-4.117	65.320	-0.009	0.000	-0.001	0.001	0.002	0.003	0.005	0.006
600	30.570	450.000	-4.857	107.249	-0.008	-0.004	-0.006	-0.007	-0.006	-0.008	-0.007	-0.007
	28.998	450.000	-4.697	113.030	0.006	-0.002	0.004	-0.002	0.003	0.000	0.003	0.002
700	29.784	450.000	-4.777	110.051	-0.009	-0.002	-0.002	-0.001	0.001	0.002	0.006	0.008
	26.640	397.385	-4.523	102.158	0.008	0.001	0.009	0.005	0.012	0.011	0.016	0.018
800	29.784	450.000	-4.777	110.051	-0.008	0.002	0.001	0.005	0.007	0.010	0.013	0.015
	24.283	268.968	-4.515	63.641	-0.010	0.000	-0.002	0.001	0.002	0.004	0.006	0.008
900	32.534	450.000	-5.055	100.926	-0.009	0.002	0.000	0.004	0.006	0.010	0.014	0.019
	21.925	187.816	-4.500	42.937	-0.009	-0.001	-0.004	-0.001	-0.001	0.002	0.004	0.008
1000	33.320	450.000	-5.134	98.638	-0.008	0.002	0.001	0.005	0.007	0.009	0.012	0.015
	21.532	173.547	-4.517	39.377	-0.009	-0.001	-0.004	-0.001	-0.002	-0.001	0.001	0.002
∞	11.901	44.469	-4.120	12.476	-0.002	0.007	-0.009	0.009	-0.008	0.006	-0.007	0.002
	10.149	36.653	-3.848	11.164	0.007	0.005	-0.006	0.007	-0.009	0.002	-0.010	-0.003

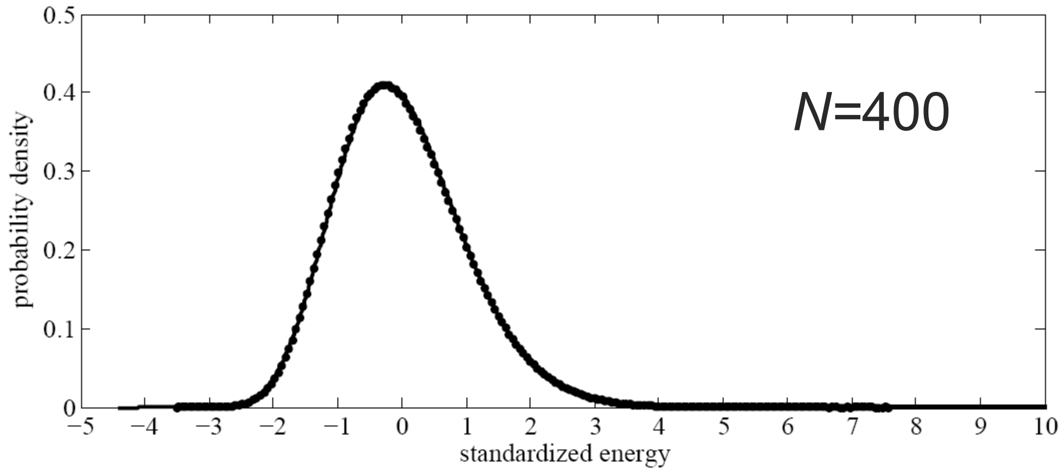
3.14 The FinisTerrae challenge III

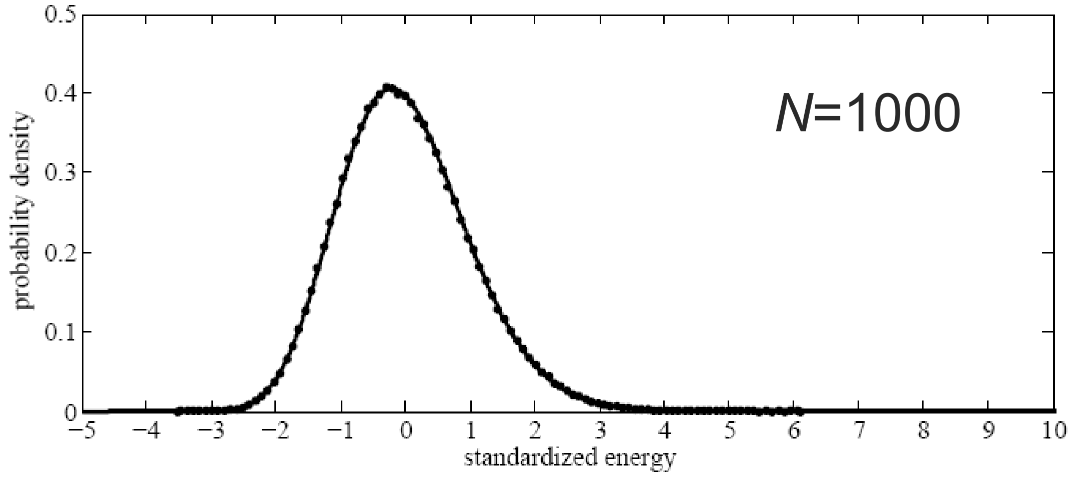
A plausible probabilistic solution: the supports.



3.15 The FinisTerrae challenge III

A plausible probabilistic solution: the histograms.





Conclusions

- We have performed in FinisTerrae different large scale experiments to study the computational complexity of the Fekete problem.
- We have obtained approximate local minima for N=10000,20000,50000. The computation times were in good agreement with the predictions.
- The experiment for $N=10^6$ confirmed the formula for the step size and corroborated the robustness of the Forces Method.
- We have collected the largest sample ever obtained for Smale's 7th problem. This has allowed us to characterize different features of the problem.
- We have shown that there exist theoretical models that adjust well all the sample information and that are compatible with the hypoyhesis of polynomial average cost, which establishes the plausibility of a probabilistic positive solution to Smale's 7th problem.

Acknowledgements

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