Genetic-algorithm energy minimization for point charges on a sphere

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(Received 20 October 1995)

We demonstrate that a recently developed approach for optimizing atomic structures is very effective for attacking the Thomson problem of finding the lowest-energy configuration of N point charges on a unit sphere. Our approach uses a genetic algorithm, combined with a ''cut and paste'' scheme of mating, that efficiently explores the different low-energy structures. Not only have we reproduced the known results for $10 \leqslant N \leqslant 132$, this approach has allowed us to extend the calculation for all $N \leqslant 200$. This has allowed us to identify series of ''magic'' numbers, where the lowest-energy structures are particularly stable. Most of these structures are icosahedral, but we also find low-energy structures that deviate from icosahedral symmetry.

A recurring problem in computational physics and chemistry is the minimization of a structure with respect to atomic positions. One difficulty is the development of an accurate model of atomic interactions in the material. However, even once such a model is chosen, optimization is often difficult, due to the many competing structures that may be locally stable. This is especially true for noncrystalline structures, such as atomic clusters and defect structures (such as grain boundaries or surfaces).[1] While accurate models of materials are becoming increasingly available, and the computational time to calculate energies is rapidly decreasing, there have been relatively few developments in the optimization process. Most efforts focus on using some form of steepest-descent or conjugate gradient relaxation, or Monte Carlo or molecular-dynamics simulations (including simulated annealing approaches).

In this paper, we use a recently developed technique[2] to study the long-standing Thomson problem of finding the lowest-energy configuration of N point charges on a unit sphere. The problem we consider here originated with Thomson's ''plum pudding'' model of the atomic nucleus. This minimization problem has been attempted by simulated annealing,[3–6] Monte Carlo approaches,[7,8] and symmetry considerations,[9] yet none of these techniques have proven as reliable as the simplest method: a repeated random search with a steepest-descent relaxation.[10–12] Thus, this problem is an ideal benchmark of new global optimization algorithms.

The energy of N point charges constrained to lie on the surface of a unit sphere is

$$E = \frac{1}{2} \sum_i \sum_{j \neq i} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}. \tag{1}$$

Even for small N, there are multiple possible stable structures; for $N \lesssim 20$, simulated annealing suffices to locate the global minimum.[3–5] However, this will not suffice once the number of local minima is large. The difficulty is that the number of metastable structures grows exponentially[10,11] with N, and these approaches do not explore different minima sufficiently rapidly once N becomes large ($N > 70$). For $N \sim 100$–110, there are ~ 50–90 metastable states;[11] this grows to $\sim$ 8000 for $N \sim$ 200. Furthermore, for many of the structures, the basin of attraction (or ''catchment region'') containing the global minimum is small compared with those of other minima.[11]

These difficulties are a generic feature of many systems, including the related problem of determining structures of atomic clusters.[2,1,13] Often, there are techniques to provide local optimization, such as steepest-descent or conjugate gradient algorithms. Monte Carlo simulations[7] and simulated annealing[3–5] are typically used to explore nearby minima, in an effort to improve upon the current minimum. The difficulty is that these techniques for ''hopping'' from one minimum to the next are time consuming, and if there are many local minima, with large barriers separating them, then these techniques are not practical. The Thomson problem is a good example of such a problem. Finding a local minimum from a random structure is straightforward, but exploring many different minima is not.

We have used a genetic algorithm[14] (GA) to tackle this problem. The idea is simple: starting with a small set of initial geometries, a number of structures that derive their properties from two of the initial geometries are generated. From this ''population,'' the lowest-energy (''most fit'') structures are chosen to replace the initial geometries. Repeating this process leads to lower-energy structures. In general, there may be other search criteria; these may be accounted for directly by constructing a ''fitness'' function that reflects the different criteria of interest, and optimizing this function by selection.[14] GA's have been applied to problems in a number of fields, but there have been few successful applications to the physical sciences.[15–18]

One of the difficulties in the type of problem that we are considering is that the evaluation of the energy is time consuming, especially for problems using more accurate models of materials. For most current applications of GA's, the computational effort in calculating the fitness is very small. Therefore, we cannot afford to use traditional approaches, which might require calculating the energies of thousands of structures, most of which would not be competitive.[16,17]

Our approach is successful because of an interesting mating algorithm[2] that allows for efficient exploration of different minima, while preserving the important properties of the parent structures. Unlike most applications of genetic algorithms,[14,16–18] our algorithm is not based upon an artifi-

TABLE I. Lowest known energies for $110<N\leqslant 200$.

N	E_1	N	E_1	N	E_1
111	5 515.293 214 59	141	9 016.615 349 19	171	13 386.355 930 72
112	5 618.044 882 33	142	9 148.271 579 99	172	13 547.018 108 80
113	5 721.824 978 03	143	9 280.839 851 19	173	13 708.635 243 04
114	5 826.521 572 16	144	9 414.371 794 46	174	13 871.187 092 30
115	5 932.181 285 78	145	9 548.928 837 23	175	14 034.781 306 94
116	6 038.815 593 58	146	9 684.381 825 58	176	14 199.354 775 65
117	6 146.342 446 58	147	9 820.932 378 38	177	14 364.850 519 22
118	6 254.877 027 79	148	9 958.406 004 27	178	14 531.309 552 93
119	6 364.347 317 48	149	10 096.859 907 40	179	14 698.754 594 23
120	6 474.756 324 98	150	10 236.196 436 70	180	14 867.099 927 53
121	6 586.121 949 58	151	10 376.571 469 28	181	15 036.467 239 78
122	6 698.374 499 26	152	10 517.867 592 88	182	15 206.730 610 91
123	6 811.827 228 17	153	10 660.082 748 24	183	15 378.166 571 04
124	6 926.169 974 19	154	10 803.372 421 14	184	15 550.421 450 32
125	7 041.473 264 02	155	10 947.574 692 28	185	15 723.720 074 08
126	7 157.669 224 87	156	11 092.803 114 78	186	15 897.897 437 05
127	7 274.819 504 68	157	11 238.903 041 16	187	16 072.975 186 32
128	7 393.007 443 07	158	11 385.990 186 20	188	16 249.250 131 48
129	7 512.107 319 27	159	11 534.023 960 96	189	16 426.371 938 87
130	7 632.167 378 91	160	11 683.054 805 55	190	16 604.445 965 00
131	7 753.205 166 94	161	11 833.084 739 47	191	16 783.452 219 37
132	7 875.045 342 80	162	11 984.050 335 81	192	16 963.338 386 46
133	7 998.179 212 90	163	12 136.013 053 22	193	17 144.564 740 88
134	8 122.089 721 19	164	12 288.930 105 32	194	17 326.616 136 47
135	8 246.909 486 99	165	12 442.804 451 37	195	17 509.489 303 93
136	8 372.743 302 54	166	12 597.649 071 32	196	17 693.460 552 12
137	8 499.534 494 78	167	12 753.469 429 75	197	17 878.382 745 77
138	8 627.406 389 88	168	12 910.212 672 27	198	18 064.288 062 96
139	8 756.227 056 95	169	13 068.006 451 13	199	18 251.082 495 64
140	8 885.980 609 04	170	13 226.681 078 60	200	18 438.842 271 98

cial ''genetic sequence'': most implementations represent the parameters of the problem symbolically as a string of numbers or characters, and then perform ''mating'' and ''mutation'' operations on a set of strings. Such an approach is inefficient for structural optimization, as many resulting structures are clearly unphysical. Instead of working with an artificial genetic sequence, we work directly with the structure itself. A new candidate structure is generated from two randomly chosen halves of two parent structures, subject to the constraint that the correct number of particles is maintained. Each candidate is then fully relaxed, using a conjugate gradient technique. By breaking with the traditional GA approaches, we are able to generate new structures that may retain the important structural features of the parents, while still being able to explore different local minima in the solution landscape. This approach has been successful for finding fullerene structures,[2] encouraging us to attempt this problem.

In the work presented here, we began with four random geometries. Using each possible each pair of initial geometries, we construct 16 more candidate structures. (Note that a cluster may ''mate'' with itself, by aligning any two randomly chosen halves of the structure.) From the 20 structures, we select the best four candidates, choosing only structures whose energies differ by more than $\Delta E=10^{-6}$ to ensure that one structure does not dominate the entire population.

For $10\leqslant N\leqslant 132$, and also for $N=192$ and $N=212$, we found the same minimum energies as given in Refs. 11 and 19. Most strikingly, for $N\leqslant 132$, we were almost always able to find the lowest-energy structures within five generations. With these successes, we went on to search for the lowest-energy structures for $133\leqslant N\leqslant 200$. The values for $111\leqslant N\leqslant 200$ are shown in Table I. We ran these for 10 generations, considering a total of 200 structures. Note that our technique does not guarantee that the lowest energy will be found, although we believe that in most cases the final structure was the global minimum. We fitted the lowest energies to the form[8,11]

$$E(N)=\frac{N^2}{2}(1-aN^{-1/2}+bN^{-3/2}). \tag{2}$$

The fitted values were $a=1.104\,61\pm 0.000\,01$ and $b=0.137\pm 0.001$, in reasonable agreement with the fit of Erber[11] and the calculations of Glasser.[8]

In Fig. 1, we show the difference between the fitted energy and the actual value for the lowest-energy structure obtained using our approach. Note that there are a series of ''magic'' numbers, with particularly low ground-state energies [relative to the trend given in Eq. (2)], for $N=12$, 32, 72, 122, 132, 137, 146, 182, and 187. In this series, the

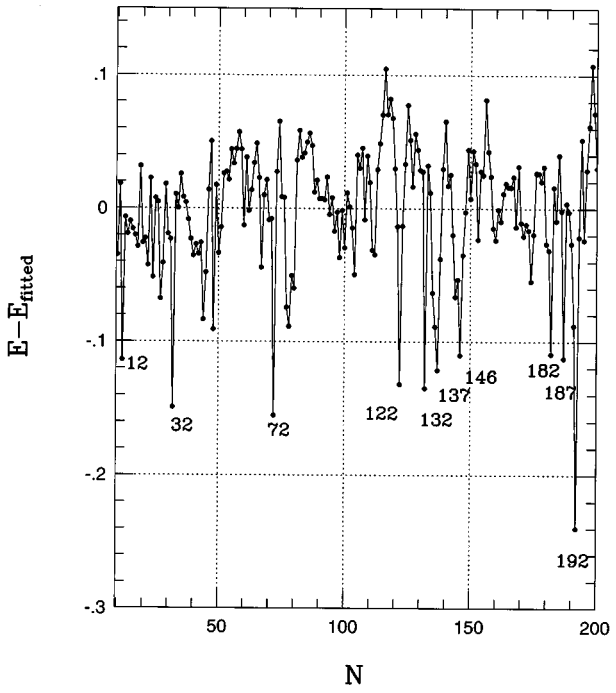

FIG. 1. We show the difference between the calculated lowest-energy configuration and the fit to the form $\frac{1}{2}N^2(1+aN^{-1/2}+bN^{-3/2})$. Note the "magic numbers" at $N=12$, 32, 72, 122, 132, 137, 146, 182, 187, and 192.

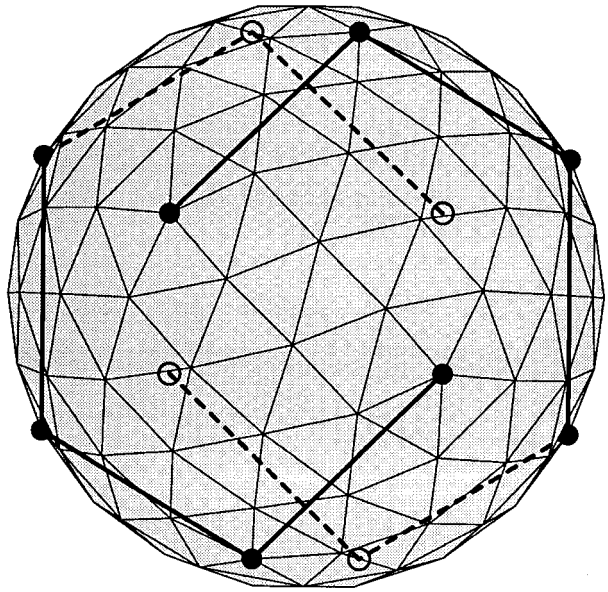

FIG. 2. This figure shows the lowest-energy structure for $N=146$, looking down one of the twofold axes. We have emphasized the fivefold coordinated charges, and indicated the interlocking C structures formed by connecting the fivefold coordinated charges to their nearest neighbor.

structures for $N=12$, 32, 72, 122, 132, and 192 have icosahedral symmetry. The icosahedral structures for $N=212$, 272, 282, and 312 also have very low energies.[19] Icosahedral structures have been predicted to have the lowest energy,[6] but for $N=42$, 92, and 162, the icosahedral structures have high energies relative to the trend in Eq. (2).

For most of the lowest-energy structures we found, the atoms tend to arrange themselves in a triangular configuration, with twelve points that have five near neighbors, and the rest having six neighbors (see Fig. 2). With this type of configuration, the application of Euler's formula predicts that the number of faces will be $F=2N-4$. This prediction is confirmed for most of the lowest-energy structures, with some exceptions (see Ref. 11). (The exceptions demonstrate that not all structures can be uniquely decomposed into triangles—on some structures, there are rectangular faces. This counterintuitive result illustrates the difficulties in making general statements concerning this problem.) The fivefold coordinated points tend to separate themselves—suggesting that the icosahedral structures would be particularly stable, with each of the fivefold coordinated points located along a line of fivefold rotational symmetry.

The striking result is that this technique can find the lowest-energy configurations, both for the high-symmetry icosahedral structures and also for structures with lower symmetry. The structures for $N=137$, 182, and 187 are distorted icosahedral structures, with D_5 symmetry. The $N=146$ structure, shown in Fig. 2, has D_2 symmetry, much lower than the symmetries of the other magic numbers. Unlike many of the structures, in which the fivefold coordinated charges form equilateral triangles, the fivefold coordinated points are not in an icosahedral arrangement. Instead, the lines connecting fivefold coordinated atoms along the shortest distance between them produce two interlocking C structures. To our knowledge, no other similar structure has been predicted as being particularly favorable. We believe that there will be other magic numbers with similar structures at larger N, and are currently exploring this.

It may seem surprising that such a simple approach works where more complicated schemes have not. We believe that there are two principal features of our technique that are important. First, we try many different geometries in parallel rather than exploring phase space in a single series of geometries. Simulated annealing or other techniques may explore several different local minima with a reasonable computational effort, but for problems with many minima, these approaches becomes impractical. This is why a simple random search is more successful than these approaches. Second, unlike a random search or more traditional approaches to genetic algorithms, our technique of generating new structures preserves much of the previous structural optimization that has occurred. The two halves remain reasonably intact, while "healing" occurs near the joining region. Thus, while we rapidly explore other minima, we do so with a bias toward the types of low-energy structures that have already been obtained.

We believe that these results are an important test of our optimization technique; they reliably reproduce all of the known low-energy structures. Our mating algorithm is easily implemented, computationally efficient, and capable of finding unusual structures. We are currently applying similar techniques to more realistic atomic models, including Lennard-Jones and embedded atom clusters, and are exploring ways of optimizing our approach. GA's have been previ-

ously proven useful in many areas, but have not been as popular or successful in the physical sciences.[15–18] We believe that successes such as ours will allow the strengths of GA's to become an effective tool in the physical sciences.

We would like to thank T. Erber for communicating his results concerning this problem prior to publication. Ames Laboratory is operated for the U.S. Department of Energy by Iowa State University under Contract No. W-7405-Eng-82. This work was supported by the Director for Energy Research, Office of Basic Energy Sciences, and the High Performance Computing and Communications initiative.

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