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FRONTIER ESTIMATORS FOR THE ASSUMED CONSECUTIVE CLUSTERS OF OPTIMUM GLOBAL POTENTIAL

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Abstract: For the first time, boundary estimators are presented for consecutive clusters of particles that possibly correspond to global potential minima where the potential depends on the number of particles (either negative decrease as with the Lennard Jones and Morse potentials, or growth positive as with the Thomson potential). Their main characteristic is that they establish that the global potential of a cluster is limited by two frontier estimators that depend on the global potentials of the previous and subsequent clusters.
This benefits global particle cluster optimization methods to distinguish solutions. Thanks to information shared on the Internet, the estimators have been successfully verified for clusters under various potentials, for example, Thomson, Lennard Jones, Morse, and for Quantum Lennard Jones for xenon, argon and neon. New Morse results are reported by verifying that previously reported results did not satisfy these estimators.
Keywords: Global Optimization, Clusters of atoms and molecules, Chemistry of materials, Nanochemistry, Molecular dynamics.

INTRODUCTION

The algorithms and programs for searching for clusters of minimum or maximum global potential constitute and are important tools in Chemistry and Physics for the study of particle clusters from the point of view of their pairwise interaction potentials. The interest in this topic is due to the predictive capacity of the models as a precedent to costly laboratory experiments, for example, for the Jones (LJ) and Morse clusters see Cambridge Cluster Database (CCD), Wales et al., 1995 and experimentally Xenon clusters have been created Echt et al. (1981), Sodium clusters by Haberland et al. (2005), some of which are related to the so-called magic numbers, and the artificial icosahedral crystals created by Noya et al. (2021). There is abundant literature and without prejudice to other research mentioned on the Lennard Jones and Morse clusters (Hartke, 2002; Morse, 1929; Hoare & McInnes, 1983; Northby, 1987; Gómez & Barrón-Romero, 1991; Maier et al., 1992; Maranas & Floudas, 1994; Deaven & Ho, 1995; Barrón et al., 1997; Leary, 1997; Wales & Doye, 1997; Doye, 1998; Wolf & Landman, 1998; Leary, 1999; Hartke, 1999; Barrón et al., 1999; Wille, 1999; Solov'yov et al., 2003; Jiang et al., 2003; Huang et al., 2002; Cai et al., 2002a; Cai et al., 2002b; Shao et al., 2004a; Xiang et al., 2004b; Xiang et al., 2004a; Shao et al., 2004b; Barrón, 2005; Shao et al., 2005; Doye, 2006; Dittner & Hartke, 2016; Barrón, 2022).

There are several ways to improve the potential of clusters, and many authors have proposed ad-hoc strategies to determine a possible optimal cluster using the previous and next cluster without explicit limits. It was Northby, in his seminal article [Northby, 1987], who expounded the concept of increasing sequence in the IC network. Similarly, other authors and in particular [Hoare and McInnes, 1983] suggested starting from the nucleus seen as the seed structure for the growth of consecutive clusters. Therefore, the increasing sequence also relates to the concept of cluster families. In [Dittner and Hartke, 2016] there is a method for kernel analysis of optimal LJ clusters using common neighbor analysis (CNA). There are a huge number of articles on the physicochemistry of the study of clusters, their importance for modern technology, the design of new materials, experimental construction and their use to understand and improve physics-inspired mathematical processes that keep this topic in focus. the frontier of scientific and technological research [Niroomand et al., 2023], [Noya et al., 2021] [Baletto and Ferrando, 2005].

Recently, the monotonicity test proposed in (Kiessling, 2023) for the possible global optimal clusters of the Lennard Jones potential motivated the search for estimators that delimit the putative and consecutive clusters of global optimal potential. To the best of my knowledge, this is the first time that frontier estimators for global optimization problems are presented under the condition that the change of potential with respect to the number of particles is linear.

METHODOLOGY

The interaction potentials for pairs of particles can be positive or negative ([Pardalos et al., 1994], for example: Born-Meyer, Kihara, LJ, Mie, Morse and Thomson potentials) and the problem can be to determine a Optimal cluster can be maximization or minimization. Without loss of generality, an increasing positive potential (P) can be assumed with respect to the number of particles and with the objective of determining the global minimum potential configuration. For example, the Thomson electrostatic potential to determine the minimum electrostatic potential over all n-electron configurations on the unit sphere is:

$$T(n) = \min_{n} \sum_{1 \le i < j \le n} T(i,j)$$

where $T(i,j) = \frac{1}{r_{ij}}$, $r_{ij} = |r_i - r_j|$ is the distance on the sphere of the electrons *i* and *j*.

In general, the potential of a cluster is:

$$P(n) = \min_{n} \sum_{1 \le i < j \le n} P(i,j)$$

where P(i,j), is the potential of the particles: *i* and *j*.

Examples of potentials that meet the properties of a potential well (Pardalos et al., 1994) are Lennard Jones (LJ) y Morse (MO):

$$\mathrm{LJ}(d_{i,j}) = \frac{1}{d_{i,j}^{12}} - \frac{2}{d_{i,j}^{6}} \quad \text{y}$$
$$\mathrm{MO}(\delta, d_{i,j}) = e^{\delta(1-d_{i,j})}(e^{\delta(1-d_{i,j})} - 2)$$

Where: $d_{i,j}$ is the Euclidean distance between the particles: *i* and *j*; y δ is the parameter for the width of the Morse potential well.

Note that in general for any pairwise potential the cluster potential corresponds to the complete graph between all the vertices and that the number of edges is the number of contributions to the potential, i.e., the number of the pairs of vertices *P(i,j)* to the potential of the cluster ands $\binom{n}{2} = \frac{n(n-1)}{2}$. Furthermore, the factor$\binom{n}{2}$, it is used in the average potential for a cluster of size: $\bar{P}(n) = \frac{2P(n)}{n(n-1)}$.

The problem of consecutive particle clusters is stated as follows: Given the possible optimal cluster of n-1 particles with potential: *P* (*n* - 1), determine the possible optimal cluster of n particles (growth).

1. 2) Or, given the possible optimal cluster of n+1 particles with potential
2. *P* (*n* - 1), determine the possible optimal cluster of *n* particles (decrease).

From the above, with good strategies to determine the intermediate cluster by growth or decrease, it must be fulfilled by construction that

$$P(n-1) < P(n) < P(n+1).$$

The above expression is the order relation of consecutive clusters that all possible optimal consecutive clusters must satisfy and that most, if not all, global optimization researchers on this topic have always used.

Proposition. For any of the supposedly optimal global potential clusters of size: n ≥ 2, is fulfilled:

$$\bar{P}(n) < \bar{P}(n+1).$$

Demonstration. Assuming the opposite, we arrive at the contradiction that: .

$$P(n) > P(n+1).$$

The two frontier estimators presented improve the order relationship by closing the interval of the potential of *P(n)* with respect to its immediate neighbors.

Proposition: For any of the supposedly optimal global potential clusters of size: n ≥ 3, is fulfilled:

$$\frac{n}{n-2}P(n-1) < P(n) < \frac{n-1}{n+1}P(n+1)$$

where *P(n - 1), P(n)* y *P(n + 1)* are the possible optimal potentials of clusters of *n* - 1, *n* y *n* + 1 particles respectively.

Demonstration. The average contribution for a cluster of size: *n* is

$$\bar{P}(n) = \frac{2P(n)}{n(n-1)}.$$

If you have: $\bar{P}$ (*n* - 1) < $\bar{P}$ (*n*) < $\bar{P}$ (*n* + 1).

To *n* - 1 y *n*:

$$\frac{2P(n-1)}{(n-1)(n-2)} < \frac{2P(n)}{n(n-1)}.$$

Simplifying: $\frac{n}{n-2}P(n-1) < P(n)$.

To *n* + 1 y *n*:

$$\frac{2P(n)}{n(n-1)} < \frac{2P(n+1)}{(n+1)n}.$$

Finally, $P(n) < P(n+1)\frac{n-1}{n+1}$.

Note that the factors of the estimators satisfy that $1<\frac{n}{n-2}$ y $\frac{n-1}{n+1}<1$ therefore, they improve the order relationship of consecutive clusters by closing the potential interval of the possible global optimal cluster of n particles.

Additionally, you have:

$$\frac{P(n-1)}{P(n+1)} < \frac{(n-1)(n-2)}{n(n+1)}.$$

Which leads to $\frac{P(n-1)}{P(n+1)}$ is increasing and asymptotically tends to 1,for example: 1.

$$\lim_{n\to\infty}\frac{P(n-1)}{P(n+1)} = 1.$$

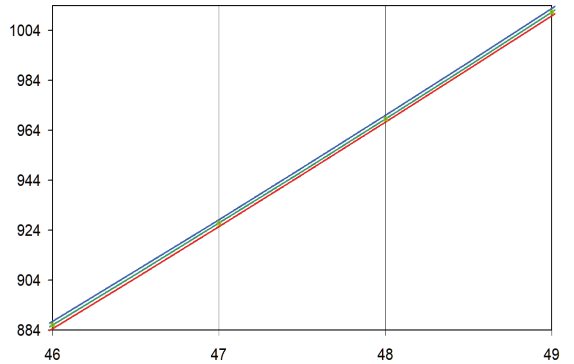

Figure 1: Example of the estimators: $\frac{n}{n-2}P(n-1)$ (red), $\frac{n-1}{n+1}P(n+1)$ (blue) around *P* (*n*) (green, reference potential) where P is the Thomson potential with 46 ≤ *n* ≤ 49.

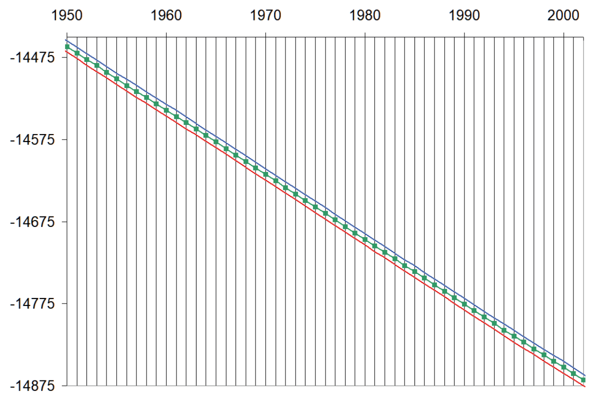

Figure 2: Example of estimators: $\frac{n}{n-2}P(n-1)$ (red), $\frac{n-1}{n+1}P(n+1)$ (blue) around *P*(*n*) (green, reference potential) where P is the LJ potential for 1950 ≤ *n* ≤ 2002.

RESULTS

Figures 1 and 2 show graphical examples of the estimators for the Thomson and LJ potentials. The following Tables show that the new frontier estimators are satisfied for the possible optimal clusters of various potentials whose data were taken from the Internet.

	n/(n-2) LJ(n-1)	LJ(n)	(n-1)/(n+1) LJ(n+1)		n/(n-2) Xe(n-1)	Xe(n)	(n-1)/(n+1) Xe(n+1)
30		-128.2866		30		-123.2835	
31	-137.1339	-133.5864	-130.9083	31	-131.7858	-128.1044	-125.5577
32	-142.4922	-139.6355	-136.0644	32	-136.6447	-133.9283	-130.5109
33	-148.6443	-144.8427	-141.2184	33	-142.5688	-138.9310	-135.4622
34	-153.8954	-150.0445	-146.8563	34	-147.6142	-143.9285	-140.8902
35	-159.1381	-155.7566	-152.8351	35	-152.6515	-149.4290	-146.6468
36	-164.9188	-161.8254	-158.0048	36	-158.2189	-155.2731	-151.6135
37	-171.0725	-167.0337	0.0000	37	-164.1458	-160.2772	
65		-334.9715		65		-322.1049	
66	-345.4394	-334.9715	-330.9282	66	-323.8115	-328.0173	-332.1706
67	-345.2783	-341.1106		67	-338.1101	-333.9306	
75		-397.4923		75		-382.1103	
76	-408.2354	-402.8949	-398.4580	76	-392.4376	-387.3240	-383.0620
77	-413.6387	-409.0835	-404.1586	77	-397.6526	-393.2770	-388.8650
78	-419.8489	-414.7944	-411.1321	78	-403.6264	-399.0983	-395.6011
79	-425.5683	-421.8109		79	-409.4645	-405.8764	
82		-440.5504		82		-423.8174	
83	-451.4282	-446.9241	-441.8797	83	-434.2820	-429.9633	-425.1124
84	-457.8247	-452.6572	-448.2545	84	-440.4502	-435.4810	-431.4236
85	-463.5646	-459.0558	-454.5616	85	-445.9745	-441.8194	-437.4118
86	-469.9857	-465.3845	-461.2453	86	-452.3389	-447.8263	-443.7837
87	-476.3347	-472.0982	-468.1455	87	-458.3634	-454.2257	-450.4297
88	-483.0772	-479.0326	-475.1314	88	-464.7891	-460.9048	-457.1789
89	-490.0449	-486.0539	-481.4909	89	-471.5003	-467.6888	-463.3120
90	-497.1006	-492.4339		90	-478.3181	-473.8418	

Table 1. Data from https://www-wales.ch.cam.ac.uk/~florent/LJZPE/table.html, Calvo, et.al. (2001) for LJ and Xenon quantum clusters.

	n/(n-2) Ar(n-1)	Ar(n)	(n-1)/(n+1) Ar(n+1)		n/(n-2) Ne(n-1)	Ne(n)	(n-1)/(n+1) Ne(n+1)
30		-113.2773		30		-80.8072	
31	-121.0895	-117.7054	-115.1685	31	-86.3801	-84.1779	-82.7148
32	-125.5524	-122.8464	-119.4391	32	-89.7898	-88.2292	-85.9020
33	-130.7720	-127.1449	-123.9497	33	-93.9214	-91.4441	-88.8603
34	-135.0914	-131.6966	-128.9581	34	-97.1593	-94.4140	-92.7399
35	-139.6782	-136.7737	-134.2702	35	-100.1361	-98.3605	-95.7781
36	-144.8192	-142.1685	-138.8309	36	-104.1464	-101.4121	-98.6572
37	-150.2924	-146.7641		37	-107.2071	-104.2947	
65		-296.3752		65		-212.7637	
66	-305.6369	-301.8306	-298.1179	66	-219.4125	-216.9323	-214.5448
67	-311.1176	-307.2907		67	-223.6072	-221.1462	
75		-351.3463		75		-253.8125	
76	-360.8421	-356.7072	-352.7499	76	-260.6723	-257.8744	-255.3315
77	-366.2194	-362.1565	-358.2777	77	-264.7510	-262.1403	-259.3953
78	-371.6870	-367.7061	-364.5389	78	-269.0387	-266.2215	-263.6360
79	-377.2569	-374.0075		79	-273.1363	-270.4836	
82		-390.5145		82		-283.2067	
83	-400.1568	-396.0417	-391.5778	83	-290.1995	-287.1670	-284.2758
84	-405.7013	-401.1284	-397.7620	84	-294.1711	-291.2094	-288.3699
85	-410.7942	-407.3466	-403.3986	85	-298.2265	-295.3186	-292.8556
86	-417.0453	-413.0033	-409.0141	86	-302.3499	-299.8284	-297.3600
87	-422.7210	-418.6380	-414.9980	87	-306.8831	-304.3567	-300.8324
88	-428.3737	-424.6491	-421.2740	88	-311.4347	-307.8285	-305.4956
89	-434.4111	-430.9584	-426.9542	89	-314.9050	-312.5185	-309.4148
90		-436.6577		90	-319.6212	-316.4470	

Table 2. Data from https://www-wales.ch.cam.ac.uk/~florent/LJZPE/table.html, Calvo, et.al. (2001) for the Argon and Neon quantum clusters.

	n/(n-2) T(n-1)	T(n)	(n-1)/(n+1) T(n+1)		n/(n-2) T(n-1)	T(n)	(n-1)/(n+1) T(n+1)
2		0.5000		55	1,286.1298	1,287.7727	1,289.3416
3	1.5000	1.7321	1.8371	56	1,335.4680	1,337.0949	1,338.7031
4	3.4641	3.6742	3.8848	57	1,385.7166	1,387.3832	1,389.0107
5	6.1237	6.4747	6.6569	58	1,436.9326	1,438.6183	1,440.2386
6	9.7120	9.9853	10.3236	59	1,489.0961	1,490.7733	1,492.3694
7	13.9794	14.4530	14.7565	60	1,542.1793	1,543.8304	1,545.5503
8	19.2706	19.6753	20.0355	61	1,596.1636	1,597.9418	1,599.5898
9	25.2968	25.7600	26.1736	62	1,651.2066	1,652.9094	1,654.6295
10	32.2000	32.7169	33.2153	63	1,707.1032	1,708.8797	1,710.6212
11	39.9874	40.5965	40.9710	64	1,764.0048	1,765.8026	1,767.5551
12	48.7157	49.1653	49.7989	65	1,821.8598	1,823.6680	1,825.3978
13	58.1044	58.8532	59.4055	66	1,880.6576	1,882.4415	1,884.1489
14	68.6621	69.3064	69.9142	67	1,940.3628	1,942.1227	1,943.9666
15	79.9689	80.6702	81.2977	68	2,000.9749	2,002.8747	2,004.6919
16	92.1946	92.9117	93.5739	69	2,062.6620	2,064.5335	2,066.3266
17	105.2999	106.0504	106.7417	70	2,125.2551	2,127.1009	2,128.9415
18	119.3067	120.0845	120.8695	71	2,188.7560	2,190.6499	2,192.3623
19	134.2121	135.0895	135.7934	72	2,253.2399	2,255.0012	2,257.0549
20	150.0994	150.8816	151.6758	73	2,318.5224	2,320.6339	2,322.5575
21	166.7638	167.6416	168.4432	74	2,385.0959	2,387.0730	2,388.9198
22	184.4058	185.2875	186.1971	75	2,452.4722	2,454.3697	2,456.2887
23	202.9340	203.9302	204.7348	76	2,520.7040	2,522.6749	2,524.5294
24	222.4693	223.3471	224.3077	77	2,589.9462	2,591.8502	2,593.7889
25	242.7686	243.8128	244.7385	78	2,660.0567	2,662.0465	2,664.0522
26	264.1305	265.1333	266.0209	79	2,731.1905	2,733.2484	2,735.2220
27	286.3440	287.3026	288.3136	80	2,803.3316	2,805.3559	2,807.4482
28	309.4028	310.4915	311.5562	81	2,876.3775	2,878.5228	2,880.5558
29	333.4909	334.6344	335.6303	82	2,950.4859	2,952.5697	2,954.5760
30	358.5369	359.6039	360.6579	83	3,025.4726	3,027.5285	3,029.5731
31	384.4042	385.5308	386.4949	84	3,101.3706	3,103.4651	3,105.5294
32	411.2329	412.2613	413.5250	85	3,178.2474	3,180.3614	3,182.4392
33	438.8588	440.2041	441.3222	86	3,256.0843	3,258.2116	3,260.2881
34	467.7168	468.9049	470.0802	87	3,334.8754	3,337.0008	3,339.0675
35	497.3233	498.5699	499.7267	88	3,414.6054	3,416.7202	3,418.8449
36	527.8975	529.1224	530.3152	89	3,495.2655	3,497.4390	3,499.5559
37	559.3580	560.6189	561.8260	90	3,576.9263	3,579.0912	3,581.2365
38	591.7644	593.0385	594.2665	91	3,659.5202	3,661.7137	3,663.8723
39	625.0946	626.3890	627.6415	92	3,743.0851	3,745.2916	3,747.4821
40	659.3569	660.6753	661.9696	93	3,827.6057	3,829.8443	3,832.0048
41	694.5561	695.9167	697.2172	94	3,913.1018	3,915.3093	3,917.5239
42	730.7126	732.0781	733.4145	95	3,999.5095	4,001.7717	4,003.9633
43	767.7892	769.1908	770.4845	96	4,086.9158	4,089.1540	4,091.3989
44	805.8190	807.1743	808.5800	97	4,175.2415	4,177.5336	4,179.7445
45	844.7173	846.1884	847.6381	98	4,264.5655	4,266.8225	4,269.1161
46	884.6515	886.1671	887.6099	99	4,354.7982	4,357.1392	4,359.3836
47	925.5523	927.0593	928.3504	100	4,446.0604	4,448.3506	4,450.6774
48	967.3662	968.7135	970.2691	101	4,538.2163	4,540.5901	4,542.8790
49	1,009.9353	1,011.5572	1,012.9750	102	4,631.4019	4,633.7366	4,636.0340
50	1,053.7054	1,055.1823	1,056.6891	103	4,725.4937	4,727.8366	4,730.1289
51	1,098.2510	1,099.8193	1,101.3644	104	4,820.5393	4,822.8765	4,825.3054
52	1,143.8121	1,145.4190	1,146.9441	105	4,916.5246	4,919.0006	4,921.3434
53	1,190.3374	1,191.9223	1,193.4592	106	5,013.5968	5,015.9846	5,018.3656
54	1,237.7655	1,239.3615	1,240.9446	107	5,111.5272	5,113.9535	5,116.2799

Table 3. Data from https://es.wikipedia.org/wiki/Problema_de_Thomson, Wikipedia (2023)

	n/(n-2) MO(3,n-1)	MO(3,n)	(n-1)/(n+1) MO(3,n+1)		n/(n-2) MO(6,n-1)	MO(6,n)	(n-1)/(n+1) MO(6,n+1)
14		-56.7547		14		-45.6193	
15	-65.4862	-63.1621	-60.4981	15	-52.6376	-49.7484	-47.1151
16	-72.1853	-69.1406	-66.7610	16	-56.8553	-53.8458	-51.1248
17	-78.3594	-75.6624	-73.4038	17	-61.0253	-57.9414	-55.7238
18	-85.1202	-82.5793	-81.1056	18	-65.1841	-62.6892	-61.2826
19	-92.2945	-90.6475	-87.6757	19	-70.0645	-68.4923	-65.2570
20	-100.7194	-97.4174	-94.4001	20	-76.1025	**-72.5078**	-69.2406
21	-107.6719	-104.3369	-101.8557	21	-80.1402	-76.5291	-73.7607
22	-114.7706	-112.0412	-110.2837	22	-84.1821	-81.1367	-79.1933
23	-122.7118	-120.7869	-117.2275	23	-88.8640	-86.7355	-83.1283
24	-131.7675	-127.8845	-125.1869	24	-94.6205	-90.6854	-87.5177
25	-139.0049	-136.0727	-134.1435	25	-98.5711	-95.1279	-92.8150
26	-147.4121	-145.3221	-141.2165	26	-103.0552	-100.5496	-96.9864
27	-156.9479	-152.5139	-149.2895	27	-108.5936	-104.7453	-101.2123
28	-164.2457	-160.7734	-158.3835	28	-112.8026	-108.9978	-106.2738
29	-172.6825	**-170.1156**	-165.7401	29	-117.0717	-114.1459	-110.5373
30	-182.2667	-177.5786	-173.9853	30	-122.2992	-118.4328	-114.9314
31	-189.8255	-185.9842	-183.2517	31	-126.6006	-122.8577	-119.7857
32	-198.3832	-195.4685	-191.8324	32	-131.0483	-127.7714	-124.2700
33	-208.0793	-204.2087	-201.4761	33	-136.0147	-132.2874	-128.7506
34	-216.9718	-214.0684	-209.0988	34	-140.5554	-136.7975	-133.8453
35	-227.0422	-221.7715	-217.7022	35	-145.0883	-141.9572	-139.1941
36	-234.8168	**-230.5083**	-227.0347	36	-150.3076	-147.3820	-143.6809
37	-243.6802	-240.0081	-236.0455	37	-155.8038	-151.8912	-149.1888
38	-253.3419	-249.1592	-245.6657	38	-160.3296	-157.4771	-155.0983
39	-262.6272	**-258.9450**	-254.9750	39	-165.9894	-163.4820	-159.5934
40	-272.5736	-268.3948	-264.8248	40	-172.0863	-167.9931	-164.1109
41	-282.1586	-278.4056	-274.6052	41	-176.6081	-172.5268	-169.2193
42	-292.3259	-288.3354	-284.3040	42	-181.1532	-177.6802	-174.5768
43	-302.4006	-298.1724	-294.2644	43	-186.3475	-183.0927	-179.0978
44	-312.3711	-308.2770	-304.4980	44	-191.8114	-187.6263	-184.3790
45	-322.6155	-318.6607	-312.8143	45	-196.3531	-192.9547	-190.5178
46	-333.1452	-327.0331	-322.3400	46	-201.7254	-199.1778	-195.0359
47	-341.5679	-336.6662	-332.2185	47	-208.0301	-203.7042	-200.3338
48	-351.3038	-346.6628	-341.8654	48	-212.5609	-209.0440	-206.4678
49	-361.4144	**-356.4128**	-351.9702	49	-217.9395	-215.2537	-211.0274

Table 4. Data from http://doye.chem.ox.ac.uk/jon/structures/Morse/tables.html, Doye et al. (1995) for Morse clusters with δ=3 and δ=6. Those marked in bold are new results.

	n/(n-2) MO(10,n-1)	MO(10,n)	(n-1)/(n+1) MO(10,n+1)		n/(n-2) MO(14,n-1)	MO(14,n)	(n-1)/(n+1) MO(14,n+1)
14		-42.6752		14		-40.7983	
15	-49.2406	-46.5414	-43.9792	15	-47.0750	-44.8064	-42.7127
16	-53.1902	-50.2619	-47.6326	16	-51.2074	-48.8145	-46.6082
17	-56.9635	-53.9836	-51.2508	17	-55.3231	-52.8226	-50.5164
18	-60.7315	-57.6571	-55.6230	18	-59.4254	-56.8309	-54.4111
19	-64.4403	-62.1668	-59.1112	19	-63.5169	-60.8124	-58.3128
20	-69.0743	-65.6791	-62.8356	20	-67.5694	-64.7920	-62.2328
21	-72.5927	-69.4499	-66.8130	21	-71.6122	-68.7836	-66.1743
22	-76.3949	-73.4943	-71.5145	22	-75.6619	-72.7917	-70.5805
23	-80.4937	-78.3254	-75.5060	23	-79.7243	-77.3025	-74.5337
24	-85.4459	-82.3702	-80.0305	24	-84.3300	-81.3095	-78.6392
25	-89.5328	-86.9897	-84.3418	25	-88.3799	-85.4774	-83.2715
26	-94.2388	-91.3703	-88.3514	26	-92.6005	-90.2108	-87.2406
27	-98.6799	-95.4195	-92.8649	27	-97.4276	-94.2198	-91.3080
28	-102.7595	-100.0084	-96.8755	28	-101.4675	-98.3317	-95.6867
29	-107.4164	-104.0514	-101.3331	29	-105.6155	-102.7746	-99.7134
30	-111.4837	-108.5712	-105.7715	30	-110.1156	-106.8358	-104.5503
31	-116.0588	-113.0661	-109.9541	31	-114.2038	-111.7607	-108.5321
32	-120.6039	-117.2843	-114.7634	32	-119.2114	-115.7676	-113.4237
33	-124.8511	-122.1675	-118.7931	33	-123.2364	-120.7413	-117.4101
34	-129.8029	-126.2177	-123.7730	34	-128.2877	-124.7483	-122.3238
35	-133.8672	-131.2744	-127.7979	35	-132.3088	-129.7374	-126.3144
36	-138.9965	-135.3154	-132.7732	36	-137.3690	-133.7447	-131.2108
37	-143.0477	-140.3602	-138.1735	37	-141.3872	-138.7086	-136.7252
38	-148.1580	-145.8498	-142.2007	38	-146.4146	-144.3211	-140.7209
39	-153.7336	-149.8872	-146.2283	39	-152.1222	-148.3274	-144.7171
40	-157.7760	-153.9245	-150.7880	40	-156.1341	-152.3337	-148.9928
41	-161.8181	-158.5207	-154.8246	41	-160.1457	-156.6335	-152.9914
42	-166.4467	-162.5658	-159.8072	42	-164.4652	-160.6410	-157.9310
43	-170.4959	-167.6026	-163.8434	43	-168.4772	-165.6350	-161.9314
44	-175.5837	-171.6455	-168.8142	44	-173.5224	-169.6424	-166.7556
45	-179.6290	-176.6660	-173.3563	45	-177.5328	-174.5116	-170.7576
46	-184.6963	-181.2362	-177.8417	46	-182.4440	-178.5193	-175.6994
47	-189.2911	-185.7458	-183.6035	47	-186.4535	-183.5082	-181.0186
48	-193.8217	-191.5863	-187.6540	48	-191.4868	-188.8890	-185.0250
49	-199.7389	-195.6393	-192.6640	49	-196.9268	-192.8984	-190.5174

Table 5: Data from http://doye.chem.ox.ac.uk/jon/structures/Morse/tables.html, Doye et al. (1995) for Morse clusters with δ=10 and δ=14.

CONCLUSIONS AND FUTURE WORK

In addition to the results of the previous section, the estimators have been satisfactorily verified for clusters under the LJ and Morse potentials for clusters from 2 to 2063 particles, which for reasons of extension are not shown in this work.

The search for new properties that are useful for global optimization is stimulating. There is a theoretical gap in tools that support necessary and sufficient conditions for global optimization for clusters of more than 5 particles. It is well known that the only global optimal cases are for clusters of between 2 and 4 elements due to the classical first and second order optimality conditions. The global optimality of the 13-particle cluster for the LJ potential was recently demonstrated (See Barrón, 2022a).

The study of mathematical, physical and chemical conditions and properties of clusters with optimal global potential will continue due to their relevance in new nano materials technologies.

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