1

Problema

Azcapotzalco Ciencias Básicas

Determinar el mínimo potencial (V) de conjuntos de n elementos donde el potencial depende de todos los pares de elementos

$\min V_{14}$

$\min V_{15}$

…

$\min V_{n-1}$

$\min V_n$

Minimización global: sobre todas los conjuntos de tamaño n = 14,15,…,n-1,n

Posiblemente no se conocen todos los arreglos espaciales de n elementos

Difíciles de resolver

Alta complejidad

2

Resumen

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1. Los estimadores de frontera son para potenciales de partículas similares al comportamiento de decrecimiento del potencial negativo de Lennard Jones. Se incluyen potenciales positivos cuyo comportamiento es creciente.
2. Su principal característica es que establecen que el potencial global de un clúster está estrictamente limitado por dos sencillos estimadores que dependen exclusivamente de los potenciales globales de los clústeres anterior y posterior.
3. Esto beneficia a los métodos de optimización global de clústeres de partículas para distinguir soluciones.
4. Gracias a la información compartida en Internet, los estimadores se han verificado con éxito para clústeres bajo diversos potenciales, por ejemplo, de Thomson, Lennard Jones, Morse, y para Quantum Lennard Jones para xenón, argón y neón.

Palabras clave: Nano Clústeres, Optimización Global, Nano Estructuras, Clústeres de Lennard Jones, Clústeres de Morse, Clústeres de Thomson.

3

Pozo de potencial

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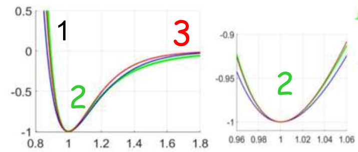


$LJ(r) = \frac{1}{r^{12}} - \frac{2}{r^6}$

$M(a,r) = e^{(a(1-r)}(e^{(a(1-r)} - 2)$

$MR(r) = M(6,r)$

$MO(r) = M(5.3554, r)$

http://www.sv.vt.edu/class/surp/surp95/Yilma/MolecDyn/lj.html

1. No se fusionan las partículas, r->0 se repelen
2. Valle de equilibrio alrededor de r*. Conjunto B (bond) aristas en (0.7,1.3). Conjunto NB de aristas-diagonales de distancia ≥ 1.3
3. Zona asintótica de baja atracción, r ≥1.3

Bonded set (B): C. D. Maranas and C. A. Floudas. Global minimum Potential Energy Conformations of Small Molecules. *Journal of Global Optimization*, 4(2):135-170, 1994.

Pozo de potencial: P. M. Pardalos, D. Shalloway, and G. L. Xue. Optimization methods for computing global minima of nonconvex potential-energy functions. *Journal of Global Optimization*, 4(2):117-133, 1994.

4

Algoritmo Evolutivo

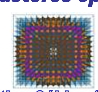
Azcapotzalco Ciencias Básicas

Fenotipo (Coordenadas de partículas)

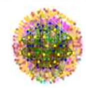
Genotipo (número de partícula)

Espacio de búsqueda

Clústeres óptimos



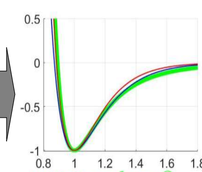
Latice Cúbica (CB½)



Latice CIF

Exploración

Fitness = Minimización



$LJ(r) = \frac{1}{r^{12}} - \frac{2}{r^6}$

$M(a,r) = e^{(a(1-r)}(e^{(a(1-r)} - 2)$

$MR(r) = M(6,r)$

$MO(r) = M(5.3554, r)$

Preservando los de mínimo potencial

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Algoritmo evolutivo

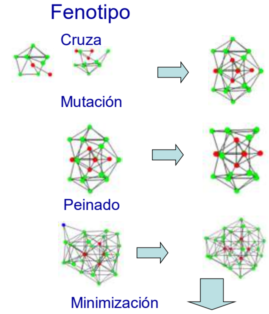
Azcapotzalco Ciencias Básicas

Fenotipo

Cruza

Mutación

Peinado



Minimización

Selección del de mínimo potencial

Orientado a la geometría

Genotipo

Combinación del DNA de clústeres o de latice

0,5,7,19,25,27,52,55,58,89,92,95,124

1, 11, 17,26,28,33,38,43,48,73,76,79, 100, 105,110,116,120,347

0, 5, 7, 19, 25, 27, 31,182, 279, 284,290, 292,295,304,314,323,332,342,348,740

0,5,7,19,25,27,52,55,58,89,92, 100, 105,110,116,120,347, 323,332,342,740

Minimización

Selección del de mínimo potencial

+ EFICIENCIA

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Minimización LBFGS

Modelo de minimización cuadrático de memoria reducida:

$$m_k(x) = f(x_k) + g_k^T(x - x_k) + 1/2\,(x - x_k)^T B_k (x - x_k)$$

donde x es el mínimo local, x_k es su aproximación, g_k gradiente, B_k es una aproximación limitada de la matriz del Hessiano de la función del problema.
Aproximación de Taylor de 2do Orden

$$LJ(x+h) = LJ(x) + \nabla LJ(x)\,h^T + 1/2 h^T \nabla^2 LJ(x)\,h + o\left(h^3\right)$$

Las soluciones cumplen:

$\nabla LJ(x^*) \approx 0$ y $LJ(x^*) \le LJ(x^* + d)$

donde $\|d\| << 1$.

J. L. Morales and J. Nocedal por algorithm 778: L-BFGS-B: Fortran subroutines for large-scale bound constrained optimization, 2011.

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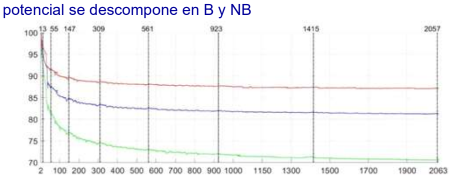
Resultados (1)
Aportación de B al PT

Conjunto B: Aristas de distancia en (0.7,1.3)

$$PT(lPT) = PT(B(lPT)) + PT(NB(lPT))$$

El potencial se descompone en B y NB



$\lim_{n\to\infty} \frac{|B(\mathrm{oPT}n)|}{|A(\mathrm{oPT}n)|} \le \lim_{n\to\infty} \frac{12n}{\binom{n}{2}} = 0.$ *A es el total de aristas*

Es importante notar que

B aporta el 70% de LJ, 83% de MO y 87% para MR

Y |B| es cada vez más insignificante que el total de aristas

CBR©

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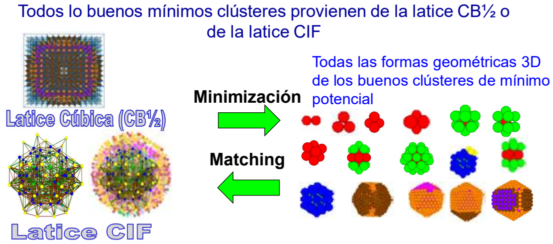
Resultados (2)

Conjetura resuelta

Todos lo buenos mínimos clústeres provienen de la latice CB½ o de la latice CIF



Hay similitudes y diferencias entre los clústeres óptimos para MR, LJ y MO

Artículo en preparación: Geometría y transformaciones entre las latices CB½ y CIF para los supuestos clústeres de mínimo potencial de Morse y LJ

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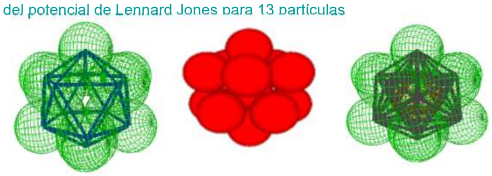
Resultados (3)

El cúmulo oLJ13_N13IC es el cúmulo mínimo global del potencial de Lennard Jones para 13 partículas



Este es el primer resultado de optimalidad global para el potencial de Lennard Jones para n > 4.

Articulo aceptado en IEEE 3rd International Conference on Electronics, Control, Optimization and Computer Science (ICECOCS) Diciembre 1-2, 2022.

CIF es completo, no hay espacio para otras configuraciones

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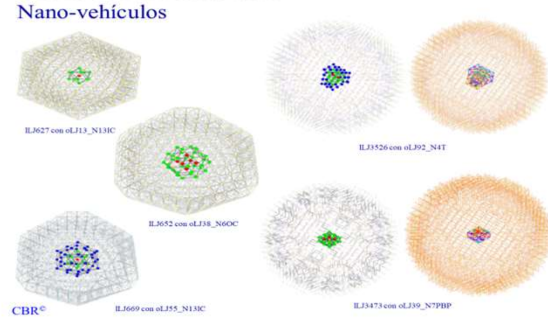
Resultados (4)

Diseño de Nanoestructuras: Nano-vehículos



Dos artículos

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11

Test de monotonía para LJ

Testing Lennard-Jones clusters for optimality

Cite as: J. Chem. Phys. 159, 014301 (2023); doi: 10.1063/5.0158931
Submitted: 18 May 2023 • Accepted: 9 June 2023 •
Published Online: 6 July 2023

Michael K.-H. Kiessling[a)]

N	$E^x(N)$	$v^x(N)$
446	−2985.461 112	−0.030 084 759 53
447	−2292.783 729	−0.023 001 211 15
448	−3000.081 058	−0.029 962 458 63

Datos actualizados

446	-2985.461112	99235	-0.030085
447	-2992.783729	99681	-0.030024
448	-3000.081058	100128	-0.029962

My thanks also go to Professor Carlos Barrón Romero for communicating his N = 447 Lennard-Jones cluster energy, for pointing out Refs. 23 and 28, and for informing me that his cluster data passed the monotonicity test of Sec. II C.

23 C. Barrón-Romero, Optimal clusters, https://academicos.azc.uam.mx/cbr/OptClusters/comMRLJMO−01.html.

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12

Estrategias para delimitar los posibles conjuntos de mínimo potencial

Se puede crear una "nube" de elementos alrededor del caso n y seleccionar el que más contribuye para crear el caso n+1.

Del caso n se puede eliminar el elemento que menos contribuye para crear el caso n-1.

Búsqueda en familias incrementando o disminuyendo elementos. Para LJ se usan N13IC, N13IR, N5BP, N7PBP, N6OC.

Era muy raro un caso anómalo en los posibles clústeres de mínimo potencial de LJ porque la gran mayoría de las implementaciones del tipo evolutivo usan las estrategias anteriores o una versión similar.

Test de monotonía para LJ


Testing Lennard-Jones clusters for optimality

Cite as: J. Chem. Phys. 159, 014301 (2023); doi: 10.1063/5.0158931
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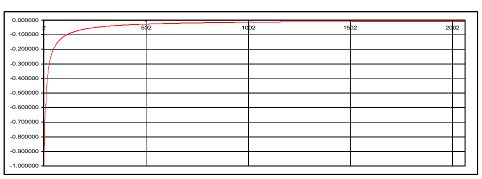
Michael K.-H. Kiessling



My thanks also go to Professor Carlos Barrón Romero for communicating his N = 447 Lennard-Jones cluster energy, for pointing out Refs. 23 and 28, and for informing me that his cluster data passed the monotonicity test of Sec. II C.

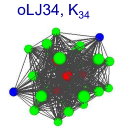
Problema de conjuntos de mínimo potencial

$$PT(C_n) = \min_{\text{todas las conf. de } n} \sum_{1\le i<j\le n} v_{ij}$$

donde $v_{ij} = V(r_{ij})$

n elementos

oLJ34, K_{34}



Un grafo completo K_n representa al conjunto de n elementos, ya que sus aristas corresponden con todas las interacciones de pares de elementos que aportan al potencial.

Una estrategia es resolver los problemas creciendo o decreciendo el número de elementos 2,3,4,…,n,

Los estimadores de frontera

Proposición. Para cualquier conjunto de supuestamente mínimo global de tamaño *n* >> 2, se cumple:

$$\frac{n+1}{n-1}\left|V\left(c_{n-1}\right)\right| \le \left|V\left(c_n\right)\right| \le \frac{n-1}{n+1}\left|V\left(c_{n+1}\right)\right|$$

donde |V(cl(•))| es potencial del conjunto respecto a todas las interacciones a pares de los elementos con crecimiento moderado menor al crecimiento lineal.

Los estimadores de frontera

Para un potencial positivo de crecimiento moderado, se tiene la desigualdad: $\left|V\left(c_{n-1}\right)\right| \lesssim \left|V\left(c_n\right)\right| \lesssim \left|V\left(c_{n+1}\right)\right|$

donde |V(cl(•))| es potencial del conjunto.

El potencial promedio de las interacciones a pares es $\dfrac{2\left|V\left(c_n\right)\right|}{n(n-1)}$

Los estimadores de frontera propuestos cierran el intervalo para tener:

$$\frac{n+1}{n-1}\left|V\left(c_{n-1}\right)\right| \le \left|V\left(c_n\right)\right| \le \frac{n-1}{n+1}\left|V\left(c_{n+1}\right)\right|$$

Ya que:

$$1 < \frac{n+1}{n-1} \qquad \frac{n-1}{n+1} < 1$$

Artículo en preparación: Frontier estimators of putatively global minimal clusters

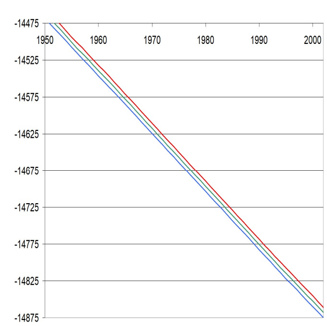
Lennard Jones 2 a 2062 partículas

C. Barrón-Romero, Optimal clusters, https://academicos.azc.uam.mx/cbr/OptClusters/comMRLJMO~01.html

	Rojo	Verde LJ	Azul
2		-1.0000	*
3	-2.0000	-3.0000	-3.0000
4	-4.5519	-6.0000	-6.0000
5	-7.6272	-9.1039	-10.0000
6	-11.0036	-12.7121	-13.6558
7	-14.1582	-16.5054	-17.7969
8	-18.0850	-19.8215	-22.0072
9	-22.1064	-24.1134	-25.4848
10	-26.2128	-28.4225	-30.1417
11	-31.0644	-32.7660	-34.7387
12	-36.9390	-37.9676	-39.3192
13	-40.4844	-44.3268	-44.8708
14	-44.8480	-47.8452	-51.7146
15	-49.2403	-52.3226	-55.2060
16	-53.6532	-56.8157	-59.7973
17	-58.7038	-61.3180	-64.3912
18	-64.5865	-66.5309	-68.9827
19	-69.0531	-72.6598	-74.3581
20	-73.5161	-77.1770	-80.7331
21	-78.5422	-81.6846	-85.3009
22	-84.4041	-86.8098	-89.8530
23	-88.8837	-92.8445	-95.0774
24	-93.8416	-97.3488	-101.2849
25	-99.6504	-102.3727	-105.8139
26	-104.1910	-108.3156	-110.9037
27	-109.0948	-112.8736	-116.9809
28	-114.7597	-117.8224	-121.5562
29	-119.4392	-123.5874	-126.5500
30	-124.6807	-128.2866	-132.4150

Se cumple hasta 2062

2050	-15235.0774	-15242.0666	-15248.8077
2051	-15243.2125	-15249.9554	-15256.9442
2052	-15250.4348	-15258.0912	-15264.8334
2053	-15257.9413	-15265.3133	-15272.9699
2054	-15265.9079	-15272.8199	-15280.1917
2055	-15273.8006	-15280.7869	-15287.6984
2056	-15281.5012	-15288.6800	-15295.6660
2057	-15289.1859	-15296.3809	-15303.5595
2058	-15296.4614	-15304.0659	-15311.2606
2059	-15304.1620	-15311.3412	-15318.9459
2060	-15311.8585	-15319.0421	-15326.2210
2061	-15319.5558	-15326.7388	-15333.9222
2062	-15327.3086	-15334.4364	-15341.6191



Morse, MO=M(5.3554,x) de 2 a 2062 partículas

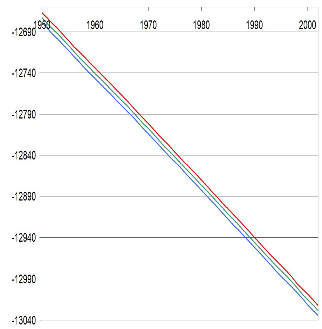
Azcapotzalco Ciencias Básicas

C. Barrón-Romero, Optimal clusters, https://academicos.azc.uam.mx/cbr/OptClusters/comMRLJMO−01.html

	Rojo	Verde MO	Azul	
2		-1.0000		*
3	-2.0000	-3.0000	-3.0000	
4	-4.5338	-6.0000	-6.0000	
5	-7.5789	-9.0676	-10.0000	
6	-10.8859	-12.6315	-13.6014	
7	-13.9399	-16.3288	-17.6841	
8	-17.7651	-19.5159	-21.7717	
9	-21.6634	-23.6868	-25.0919	
10	-25.6230	-27.8529	-29.6085	
11	-30.3591	-32.0288	-34.0425	
12	-36.0981	-37.1056	-38.4345	
13	-39.4331	-43.3177	-43.8520	
14	-43.5901	-46.6027	-50.5373	
15	-47.7560	-50.8551	-53.7724	
16	-51.9322	-55.1031	-58.1201	
17	-56.8008	-59.3511	-62.4502	
18	-62.5863	-64.3743	-66.7700	
19	-66.7712	-70.4096	-71.9477	
20	-70.9400	-74.6266	-78.2329	
21	-75.7622	-78.8222	-82.4820	
22	-81.5131	-83.7371	-86.7044	
23	-85.6708	-89.6645	-91.7121	
24	-90.3764	-93.8300	-97.8158	
25	-96.0656	-98.5924	-101.9891	
26	-100.3514	-104.4191	-106.8084	
27	-104.9325	-108.7141	-112.7727	
28	-110.4724	-113.3271	-117.0767	
29	-114.8434	-118.9703	-121.7217	
30	-119.4953	-123.3504	-127.4681	

Se cumple hasta 2062

2050	-13355.1322	-13361.6825	-13368.2328
2051	-13361.6241	-13368.1744	-13374.7246
2052	-13368.1160	-13374.6662	-13381.2165
2053	-13374.6079	-13381.1581	-13387.7083
2054	-13381.0998	-13387.6500	-13394.2002
2055	-13387.5917	-13394.1418	-13400.6920
2056	-13393.5448	-13400.6337	-13407.1838
2057	-13397.6915	-13406.5862	-13413.6757
2058	-13403.6029	-13410.7306	-13419.6276
2059	-13410.5105	-13416.6414	-13423.7698
2060	-13417.0049	-13423.5494	-13429.6800
2061	-13423.8903	-13430.0438	-13436.5883
2062	-13431.0735	-13436.9295	-13443.0827



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Morse, MR = M(6,x) de 2 a 2062 partículas

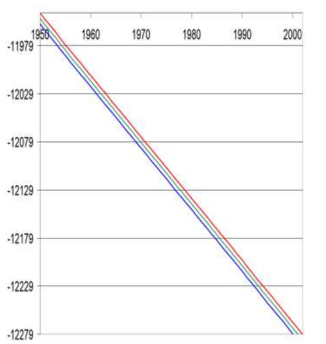
Azcapotzalco Ciencias Básicas

C. Barrón-Romero, Optimal clusters, https://academicos.azc.uam.mx/cbr/OptClusters/comMRLJMO−01.html

	Rojo	Verde MR	Azul	
2		-1.0000		*
3	-2.0000	-3.0000	-3.0000	
4	-4.5225	-6.0000	-6.0000	
5	-7.4927	-9.0449	-10.0000	
6	-10.8051	-12.4878	-13.5674	
7	-13.8053	-16.2076	-17.4829	
8	-17.5629	-19.3274	-21.6101	
9	-21.3681	-23.4172	-24.8495	
10	-25.2175	-27.4733	-29.2715	
11	-29.7820	-31.5219	-33.5785	
12	-35.3666	-36.4003	-37.8263	
13	-38.6009	-42.4399	-43.0185	
14	-42.6415	-45.6193	-49.5132	
15	-46.6664	-49.7484	-52.6376	
16	-50.6987	-53.8458	-56.8553	
17	-55.3140	-57.9414	-61.0253	
18	-60.8820	-62.6892	-65.1841	
19	-64.8754	-68.4923	-70.0645	
20	-68.8762	-72.5078	-76.1025	
21	-73.4094	-76.5291	-80.1402	
22	-78.8504	-81.1367	-84.1821	
23	-82.7997	-86.7355	-88.8640	
24	-87.2006	-90.6854	-94.6205	
25	-92.5056	-95.1279	-98.5711	
26	-96.6879	-100.5496	-103.0552	
27	-100.9239	-104.7453	-108.5936	
28	-105.9927	-108.9978	-112.8026	
29	-110.2651	-114.1459	-117.0717	
30	-114.6672	-118.4328	-122.2992	

Se cumple hasta 2062

2050	-12585.6670	-12591.6938	-12597.4253
2051	-12591.9308	-12597.9577	-12603.9843
2052	-12598.2456	-12604.2216	-12610.2484
2053	-12604.8036	-12610.5366	-12616.5124
2054	-12611.3617	-12617.0950	-12622.8276
2055	-12617.6254	-12623.6534	-12629.3864
2056	-12623.8889	-12629.9173	-12635.9452
2057	-12630.2037	-12636.1809	-12642.2092
2058	-12636.7616	-12642.4959	-12648.4729
2059	-12643.3195	-12649.0542	-12654.7880
2060	-12649.5829	-12655.6125	-12661.3467
2061	-12655.8463	-12661.8760	-12667.9054
2062	-12662.0648	-12668.1395	-12674.1691



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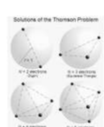
Problema de Thomson

Azcapotzalco Ciencias Básicas

https://en.wikipedia.org/wiki/Thomson_problem

Determinar mínimo potencial electrostático simplificado sobre todas las configuraciones de N electrones sobre la esfera unitaria:



$$\min_{N} \sum_{1 \le i < j \le N} \frac{1}{r_{ij}}$$

$r_{ij} = |r_i - r_j|$ Es la distancia entre los vectores sobre la esfera de los electrones *i* e *j*

El problema de Thomson está relacionado con el 7to de los 18 problemas matemáticos no resueltos propuestos por el matemático Steve Smale: "Distribución de puntos en la 2D esfera". La principal diferencia es que en el problema de Smale la función a minimizar no es el potencial electrostático sino un potencial logarítmico dado por $-\log r_{ij}$. Una segunda diferencia es que la pregunta de Smale es sobre el comportamiento asintótico del potencial total cuando el número N de puntos llega al infinito, no para valores concretos de N.

N	U_{Thom}	Symmetry	$\left\|\sum \mathbf{r}_i\right\|$	v_3	v_4	v_5	v_6	v_7	v_8	e	f_3	f_4	θ_1	Equivalent polyhedron
2	0.500000000	$D_{\infty h}$	0	–	–	–	–	–	–	2	–	–	180.000°	digon
3	1.732050808	D_{3h}	0	–	–	–	–	–	–	3	2	–	120.000°	triangle
4	3.674234614	T_d	0	4	0	0	0	0	0	6	4	0	109.471°	tetrahedron
5	6.474691495	D_{3h}	0	2	3	0	0	0	0	9	6	0	90.000°	triangular dipyramid
6	9.985281374	O_h	0	0	6	0	0	0	0	12	8	0	90.000°	octahedron
7	14.452977414	D_{5h}	0	0	5	2	0	0	0	15	10	0	72.000°	pentagonal dipyramid
8	19.675287861	D_{4d}	0	0	8	0	0	0	0	16	8	2	71.694°	square antiprism
9	25.759986531	D_{3h}	0	0	3	6	0	0	0	21	14	0	69.190°	triaugmented triangular prism
10	32.716949460	D_{4d}	0	0	2	8	0	0	0	24	16	0	64.996°	gyroelongated square dipyramid
11	40.596450510	C_{2v}	0.013219635	0	2	8	1	0	0	27	18	0	58.540°	edge-contracted icosahedron
12	49.165253058	I_h	0	0	0	12	0	0	0	30	20	0	63.435°	icosahedron (geodesic sphere {3,5+}1,0)
13	58.853230612	C_{2v}	0.008820367	0	1	10	2	0	0	33	22	0	52.317°	
14	69.306363297	D_{6d}	0	0	0	12	2	0	0	36	24	0	52.866°	gyroelongated hexagonal dipyramid

21

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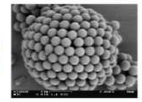
The Thomson Problem and Spherical Crystallography

1904: J. J. Thomson asks how particles pack on a sphere – relevant to viruses, colloid-coated droplets, and multielectron bubbles in helium

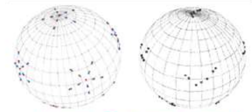
Simian virus SV40



"Colloidosome" = colloids of radius ***a*** coating water droplet (radius ***R***) -- Weitz Laboratory

- **Continuum elastic theory (with M. Bowick and A. Travesset) shows that the 5-fold disclinations become unstable to unusual *finite length* grain boundaries (strings of dislocations) for R/a >> 1.**
- **Finding the ground state of ~26,000 particles on a sphere is replaced by minimizing the energy of only ~ 250 interacting disclinations, representing points of local 5- and 7-fold symmetry.**
- **Grain boundaries in ground state for R/a > 5-10 have important implications for the mechanical stability and porosity of colloidosomes, proposed as delivery vehicles for drugs, flavors and fragrances.**

Ordering on a sphere ➔ a minimum of 12 5-fold disclinations, as in soccer balls and fullerenes -- what happens for *R/a >> 1* ?



Dislocations (5-7 defect pairs) embedded in spherical ground states

22

Configuraciones de menor energía conocidas del problema de Thomson

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https://en.wikipedia.org/wiki/Thomson_problem

		THOMSON		
2	Inferior	0.5000	Superior	
3	1.5000	1.7321	1.2247	*
4	3.4641	3.6742	3.2373	*
5	6.1237	6.4747	5.9912	*
6	9.7120	9.9853	9.6353	*
7	13.9794	14.4530	14.0538	*
8	19.2706	19.6753	19.3200	*
9	25.2968	25.7600	25.4465	*
10	32.2000	32.7169	32.4772	*
11	39.9874	40.5965	40.2261	*
12	48.7157	49.1653	49.0444	*
13	58.1044	58.8532	58.6438	*
14	68.6621	69.3064	69.1459	*
15	79.9689	80.6702	80.5234	*
16	92.1946	92.9117	92.7941	*
17	105.2999	106.0504	105.9569	*
18	119.3067	120.0845	120.0795	*
19	134.2121	135.0895	134.9993	*
20	150.0994	150.8816	150.8775	*
21	166.7638	167.6416	167.6411	*
22	184.4058	185.2875	185.3911	
23	202.9340	203.9302	203.9256	*
24	222.4693	223.3471	223.4950	
25	242.7686	243.8128	243.9227	
26	264.1305	265.1333	265.2024	
27	286.3440	287.3026	287.4922	
28	309.4028	310.4915	310.7320	

29	333.4909	334.6344	334.8037
30	358.5369	359.6039	359.8288
31	384.4042	385.5308	385.6638
32	411.2329	412.2613	412.6913
33	438.8588	440.2041	440.4864
34	467.7168	468.9049	469.2422
35	497.3233	498.5699	498.8868
36	527.8975	529.1224	529.4734
37	559.3580	560.6189	560.9824
38	591.7644	593.0385	593.4212
39	625.0946	626.3890	626.7945
40	659.3569	660.6753	661.1209
41	694.5561	695.9167	696.3670
42	730.7126	732.0781	732.5627
43	767.7892	769.1908	769.6313
44	805.8190	807.1743	807.7253
45	844.7173	846.1884	846.7819
46	884.6515	886.1671	886.7523
47	925.5523	927.0593	927.4916
48	967.3662	968.7135	969.4090
49	1009.9353	1011.5572	1012.1136
50	1053.7054	1055.1823	1055.8265
51	1098.2510	1099.8193	1100.5006
52	1143.8121	1145.4190	1146.0791
53	1190.3374	1191.9223	1192.5931
54	1237.7655	1239.3615	1240.0774
55	1286.1298	1287.7727	1288.4733
56	1335.4680	1337.0949	1337.8338

Se cumple de 57 a 189

190	16601.1206	16604.4283	16606.7843	
191	16780.1366	16783.4522	16785.7118	
192	16960.1201	16963.3384	16965.9755	
193	17140.9650	17144.5647	17147.0657	
194	17323.1540	17326.6161	17328.9791	
195	17506.1666	17509.4893	17511.9892	
196	17689.9995	17693.4605	17695.9081	
197	17874.9319	17878.3402	17880.8687	
198	18060.7722	18064.2622	18066.7281	
199	18247.6557	18251.0825	18253.5277	
200	18435.4369	18438.8427	18441.3153	
201	18624.1577	18627.5912	18629.9689	
202	18813.8671	18817.2047	18819.7834	
203	19004.4406	19007.9812	19010.3827	
204	19196.1790	19199.5408		*
255	0.0000	30264.4243		*
256	30502.7268	30506.6875	30509.7075	
257	0.0000	30749.9414		*

* No satisface 22 casos
Se satisface N=22, 24-204 y 256

23

Quantum partition functions from classical distributions. Application to rare-gas clusters

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JOURNAL OF CHEMICAL PHYSICS VOLUME 114, NUMBER 17 1 MAY 2001

Quantum partition functions from classical distributions: Application to rare-gas clusters

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(Received 5 December 2000; accepted 8 February 2001)

https://www-wales.ch.cam.ac.uk/~florent/LJZPE/table.html

		LJ		
30		-128.2866		*
31	-130.6268	-133.5864	-137.1339	
32	-135.7901	-139.6355	-142.4922	
33	-140.9509	-144.8427	-148.6443	
34	-146.5945	-150.0445	-153.8954	
35	-152.5782	-155.7566	-159.1381	
36	-157.7540	-161.8254	-164.9188	
37	0.0000	-167.0337	-171.0725	
65		-334.9715		*
66	-330.7739	-334.9715	-345.4394	
67	0.0000	-341.1106	-345.2783	
75		-397.49233		*
76	-398.3182	-402.89487	-408.2354	
77	-404.0205	-409.08352	-413.6387	
78	-410.9952	-414.7944	-419.8489	
79	0.0000	-421.8109	-425.5683	
82		-440.55043		*
83	-441.7498	-446.92409	-451.4282	
84	-448.1259	-452.65721	-457.8247	
85	-454.4343	-459.0558	-463.5646	
86	-461.1191	-465.38449	-469.9857	
87	-468.0204	-472.09816	-476.3347	
88	-475.0072	-479.03263	-483.0772	
89	-481.3680	-486.05391	-490.0449	
90	0.0000	-492.43391	-497.1006	

		XE		
30		-123.2835		*
31	-125.2877	-128.1044	-131.7858	
32	-130.2478	-133.9283	-136.6447	
33	-135.2056	-138.9310	-142.5688	
34	-140.6391	-143.9285	-147.6142	
35	-146.4003	-149.4290	-152.6515	
36	-151.3729	-155.2731	-158.2189	
37	0.0000	-160.2772	-164.1458	
65		-322.1049		
66	-323.8115	-328.0173	-332.1706	
67	0.0000	-333.9306	-338.1101	
75		-382.11032		*
76	-382.9276	-387.32395	-392.4376	
77	-388.7321	-393.27696	-397.6526	
78	-395.4693	-399.09829	-403.6264	
79	0.0000	-405.87642	-409.4645	
82		-423.81738		*
83	-424.9874	-429.9633	-434.2820	
84	-431.2999	-435.48096	-440.4502	
85	-437.2892	-441.8194	-445.9745	
86	-443.6623	-447.82634	-452.3389	
87	-450.3093	-454.22568	-458.3634	
88	-457.0595	-460.90478	-464.7891	
89	-463.1937	-467.68876	-471.5003	
90	0.0000	-473.84183	-478.3181	

		Ar		
30		-113.2773		*
31	-114.9208	-117.7054	-121.0895	
32	-119.1983	-122.8464	-125.5524	
33	-123.7150	-127.1449	-130.7720	
34	-128.7282	-131.6966	-135.0914	
35	-134.0445	-136.7737	-139.6782	
36	-138.6106	-142.1685	-144.8192	
37	0.0000	-146.7641	-150.2924	
65		-296.3752		*
66	-297.9789	-301.8306	-305.6369	
67	0.0000	-307.2907	-311.1176	
75		-351.34629		*
76	-352.6261	-356.7072	-360.8421	
77	-358.1553	-362.15653	-366.2194	
78	-364.4175	-367.70607	-371.6870	
79	0.0000	-374.00745	-377.2569	
82		-390.51446		*
83	-391.4627	-396.04172	-400.1568	
84	-397.6479	-401.12844	-405.7013	
85	-403.2856	-407.3466	-410.7942	
86	-408.9022	-413.00329	-417.0453	
87	-414.8870	-418.63798	-422.7210	
88	-421.1639	-424.64907	-428.3737	
89	-426.8451	-430.95844	-434.4111	
90	0.0000	-436.65766	-440.7530	

		Ne		
30		-80.8072		*
31	-82.5369	-84.1779	-86.3801	
32	-85.7288	-88.2292	-89.7898	
33	-88.6920	-91.4441	-93.9214	
34	-92.5746	-94.4140	-97.1593	
35	-95.6171	-98.3605	-100.1361	
36	-98.5006	-101.4121	-104.1464	
37	0.0000	-104.2947	-107.2071	
65		-212.7637		*
66	-214.4448	-216.9323	-219.4125	
67	0.0000	-221.1462	-223.6072	
75		-253.81249		*
76	-255.2419	-257.87437	-260.6723	
77	-259.3066	-262.14029	-264.7510	
78	-263.5482	-266.22148	-269.0387	
79	0.0000	-270.48364	-273.1363	
82		-283.20672		*
83	-284.1923	-287.16698	-290.1995	
84	-288.2872	-291.20937	-294.1711	
85	-292.7736	-295.31855	-298.2265	
86	-297.2786	-299.82836	-302.3499	
87	-300.7519	-304.35668	-306.8831	
88	-305.4158	-307.82846	-311.4347	
89	-309.3358	-312.51846	-314.9050	
90	0.0000	-316.44695	-319.6212	

* No satisface

24

Morse ρ = 3, 6,10 y 14

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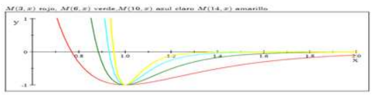
http://doye.chem.ox.ac.uk/jon/structures/Morse/tables.html



	RHO=3				RHO=6				RHO=10				RHO=14		
14		-56.7547	*	14		-45.6193	*	14		-42.6752	*	14		-40.7983	*
15	-59.9219	-63.1621	-65.4862	15	-46.6664	-49.7484	-52.6376	15	-43.5604	-46.5414	-49.2406	15	-42.3059	-44.8064	-47.0750
16	-66.2046	-69.1406	-72.1853	16	-50.6987	-53.8458	-56.8553	16	-47.2356	-50.2619	-53.1902	16	-46.2198	-48.8145	-51.2074
17	-72.8641	-75.6624	-78.3594	17	-55.3140	-57.9414	-61.0253	17	-50.8739	-53.9836	-56.9635	17	-53.6580	-52.8226	-55.3231
18	-80.5755	-82.5793	-85.1202	18	-60.8820	-62.6892	-65.1841	18	-55.2594	-57.6571	-60.7315	18	-54.0555	-60.8124	-59.4254
19	-87.1629	-90.6475	-92.2945	19	-68.4734	-68.4923	-70.0645	19	-58.7655	-62.1668	-64.4403	19	-61.5432	-60.8124	-67.9668
20	-93.9033	-97.4174	-100.7194	20	-68.8762	-76.5291	-76.1025	20	-62.5049	-65.6791	-69.0743	20	-61.9052	-68.7836	-67.5694
21	-101.3706	-104.3369	-107.6719	21	-73.4094	-76.5291	-84.5848	21	-66.4948	-69.4499	-72.5927	21	-65.8592	-68.7836	-76.0239
22	-109.8063	-112.0412	-114.7706	22	-78.8504	-81.1367	-84.1821	22	-71.2049	-73.4943	-76.3949	22	-70.2750	-72.7917	-75.6619
23	-116.7642	-120.7869	-122.7118	23	-82.7997	-86.7355	-88.8640	23	-75.2076	-78.3254	-80.4937	23	-74.2391	-77.3025	-79.7243
24	-124.7333	-127.8845	-131.7675	24	-87.2006	-90.6854	-94.6205	24	-79.7405	-82.3702	-85.4459	24	-78.3543	-81.3095	-84.3300
25	-133.6964	-136.0727	-139.0049	25	-92.5056	-95.1279	-98.5711	25	-84.0606	-86.9897	-89.5328	25	-82.9939	-85.4774	-88.3799
26	-140.7820	-145.3221	-147.4121	26	-96.6879	-100.5496	-103.0552	26	-88.0795	-91.3703	-94.2388	26	-86.9721	-90.2108	-92.6005
27	-148.8642	-152.5139	-156.9479	27	-100.9239	-104.7453	-108.5936	27	-92.6003	-95.4195	-98.6799	27	-91.0479	-94.2198	-97.4276
28	-157.9644	-160.7734	-164.2457	28	-105.9927	-108.9978	-112.8026	28	-96.6192	-100.0084	-102.7595	28	-95.4335	-98.3317	-101.4675
29	-165.3318	**-170.1156**	-172.6825	29	-110.2651	-114.1459	-117.0717	29	-101.0835	-104.0514	-107.4164	29	-99.4678	-102.7746	-105.6155
30	-173.5853	-177.5786	-182.2667	30	-114.6672	-118.4328	-122.2992	30	-105.5284	-108.5712	-111.4837	30	-104.3100	-106.8358	-110.1156
31	-182.8576	-185.9842	-189.8255	31	-119.5281	-122.8577	-126.6006	31	-109.7176	-113.0661	-116.0588	31	-108.2987	-111.7607	-114.2038
32	-191.4457	-195.4685	-198.3832	32	-124.0195	-127.7714	-131.0483	32	-114.5320	-117.2843	-120.6039	32	-113.1950	-115.7676	-119.2114
33	-201.0946	-204.2087	-208.0793	33	-128.5068	-132.2874	-136.0147	33	-118.5681	-122.1675	-124.8511	33	-117.1878	-120.7413	-123.2364
34	-208.7261	-214.0684	-216.9718	34	-133.6068	-136.7975	-140.5554	34	-123.5524	-126.2177	-129.8029	34	-122.1058	-124.7483	-128.2877
35	-217.3364	-221.7715	-227.0422	35	-138.9601	-141.9572	-145.0883	35	-127.5831	-131.2744	-133.8672	35	-126.1021	-129.7374	-132.3088
36	-226.6743	**-230.5083**	-234.8168	36	-143.4528	-147.3820	-150.3076	36	-132.5624	-135.3154	-138.9965	36	-131.0025	-133.7447	-137.3690
37	-235.6911	-240.0081	-243.6802	37	-148.9648	-151.8912	-155.8038	37	-137.9660	-140.3602	-143.0477	37	-136.5199	-138.7086	-141.3872
38	-245.3163	-249.1592	-253.3419	38	-154.8777	-157.4771	-160.3296	38	-141.9984	-145.8498	-148.1580	38	-140.5207	-144.3211	-146.4146
39	-254.6309	**-258.9450**	-262.6272	39	-159.3781	-163.4820	-165.9894	39	-146.0310	-149.8872	-153.7336	39	-144.5218	-148.3274	-152.1222
40	-264.4853	-268.3948	-272.5736	40	-163.9005	-167.9931	-172.0863	40	-150.5947	-153.9245	-157.7760	40	-148.8018	-152.3337	-156.1341

29,36 y 39 nuevos resultados CBR

Morse ρ = 3, 6,10 y 14

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http://doye.chem.ox.ac.uk/jon/structures/Morse/tables.html

41	-274.2703	-278.4056	-282.1586	41	-169.0129	-172.5268	-176.6081	41	-154.6358	-158.5207	-161.8181	41	-152.8049	-156.6335	-160.1457
42	-283.9738	-288.3354	-292.3259	42	-174.3740	-177.6802	-181.1532	42	-159.6216	-162.5658	-166.4467	42	-157.7476	-160.6410	-164.4652
43	-293.9385	-298.1724	-302.4006	43	-178.8995	-183.0927	-186.3475	43	-163.6620	-167.6026	-170.4959	43	-161.7521	-165.6350	-168.4772
44	-304.1761	-308.2770	-312.3711	44	-184.1841	-187.6263	-191.8114	44	-168.6357	-171.6455	-175.5837	44	-166.5793	-169.6424	-173.5224
45	-312.4983	-318.6607	-322.6155	45	-190.3254	-192.9547	-196.3531	45	-173.1812	-176.6660	-179.6290	45	-170.5851	-174.5116	-177.5328
46	-322.0285	-327.0331	-333.1452	46	-194.8475	-199.1778	-201.7254	46	-177.6699	-181.2362	-184.6963	46	-175.5296	-178.5193	-182.4440
47	-331.9112	-336.6662	-341.5679	47	-200.1485	-203.7042	-208.0301	47	-183.4337	-185.7458	-189.2911	47	-180.8511	-183.5082	-186.4535
48	-341.5623	-346.6628	-351.3038	48	-206.2848	-209.0440	-212.5609	48	-187.4877	-191.5863	-193.8217	48	-184.8610	-188.8890	-191.4868
49	-351.6709	**-356.4128**	-361.4144	49	-210.8480	-215.2537	-217.9395	49	-192.5001	-195.6393	-199.7389	49	-190.3554	-192.8984	-196.9268
50	-361.6065	-366.6356	-371.2634	50	-216.3756	-219.8202	-224.2226	50	-196.5548	-200.6916	-203.7910	50	-194.3695	-198.4556	-200.9358
51	-372.3878	-376.6734	-381.6003	51	-222.5321	-225.3912	-228.7925	51	-201.5694	-204.7446	-208.8831	51	-199.3443	-202.4683	-206.5559
52	-383.4454	-387.5873	-391.7403	52	-228.6875	-231.6150	-234.4069	52	-206.1632	-209.7967	-212.9344	52	-203.3590	-207.4808	-210.5670
53	-392.5711	-398.7832	-402.7868	53	-234.8484	-237.8350	-240.6980	53	-211.8122	-214.4097	-218.0241	53	-208.4619	-211.4934	-215.6173
54	-402.4401	-407.9660	-414.1210	54	-241.0167	-244.0582	-246.9825	54	-217.4508	-220.1186	-222.6562	54	-212.4741	-216.6369	-219.6278
55	-413.0254	-417.9186	-423.3610	55	-244.6894	-250.2866	-253.2679	55	-220.5765	-225.8143	-228.4250	55	-217.4495	-220.6462	-224.8118
56	-424.2475	-428.6113	-433.3970	56	-248.8259	-253.9230	-259.5565	56	-225.2434	-228.9002	-234.1778	56	-222.4260	-225.6551	-228.8183
57	-433.6627	-439.9603	-444.1972	57	-254.1683	-258.0417	-263.1565	57	-230.2849	-233.5857	-237.2238	57	-226.5702	-230.6640	-233.8608
58	-443.6641	-449.4323	-455.6732	58	-258.7057	-263.4108	-267.2575	58	-234.9398	-238.6589	-241.9280	58	-232.2769	-234.8091	-238.9020
59	-454.5011	-459.5093	-465.2018	59	-264.0754	-267.9452	-272.6532	59	-239.3865	-243.3305	-247.0329	59	-236.2883	-240.5725	-243.0480
60	-465.9582	-470.4485	-475.3544	60	-269.4357	-273.3412	-277.1847	60	-244.0721	-247.7860	-251.7212	60	-241.2681	-244.5791	-248.8681
61	-474.9523	-482.0258	-486.3959	61	-273.8983	-278.7266	-282.6070	61	-248.4850	-252.4883	-256.1855	61	-245.2978	-249.5877	-252.8699
62	-485.5470	-491.0524	-498.0933	62	-279.2525	-283.1830	-288.0175	62	-253.5774	-256.9082	-260.9046	62	-250.2780	-253.6129	-257.9073
63	-496.5513	-501.7319	-507.1525	63	-284.6006	-288.5609	-292.4677	63	-259.5151	-262.0300	-265.3314	63	-256.1875	-258.6206	-261.9281
64	-507.0887	-512.8317	-517.9168	64	-289.0676	-293.9317	-297.8694	64	-263.5957	-268.0238	-270.4826	64	-260.2011	-264.5870	-266.9632
65	-518.0190	-523.4464	-529.1121	65	-294.4167	-298.3923	-303.2629	65	-268.6177	-272.0988	-276.5325	65	-265.1838	-268.5947	-272.9866
66	-528.2466	-534.4640	-539.8041	66	-299.7627	-303.7633	-307.7171	66	-273.6209	-277.1452	-280.6019	66	-269.9646	-273.6023	-276.9883
67	-538.9979	-544.7543	-550.9091	67	-304.9906	-309.1303	-313.1099	67	-278.0868	-282.1716	-285.6728	67	-274.2447	-278.4010	-282.0209
68	-549.7064	-555.5825	-561.2620	68	-310.4134	-314.3749	-318.4979	68	-282.7266	-286.6433	-290.7222	68	-279.0073	-282.6830	-286.8373
69	-560.9937	-566.3641	-572.1670	69	-316.4417	-319.8199	-323.7592	69	-287.8205	-291.2941	-295.1998	69	-283.9857	-287.4621	-291.1213
70	-571.5854	-577.7398	-583.0219	70	-322.1148	-325.8877	-329.2264	70	-293.7652	-296.4121	-299.8615	70	-289.8795	-292.4629	-295.9169
71	-582.7976	-588.3967	-594.4859	71	-326.6535	-331.5887	-335.3338	71	-297.8275	-302.4054	-305.0038	71	-293.8945	-298.4054	-300.9400
72	-593.9662	-599.6903	-605.2080	72	-331.7866	-336.1218	-341.0627	72	-302.8643	-306.4602	-311.0455	72	-298.8816	-302.4132	-306.9312
73	-605.6201	-610.9367	-616.5830	73	-337.1146	-341.2663	-345.5900	73	-307.9754	-311.5175	-315.0929	73	-303.8813	-307.4211	-310.9319
74	-616.3914	-622.6799	-627.9071	74	-341.9731	-346.6108	-350.7459	74	-313.9235	-316.6508	-320.1708	74	-309.8017	-312.4413	-315.9606
75	-627.7529	-633.5134	-639.7396	75	-346.8694	-351.4724	-356.1070	75	-317.9856	-322.6436	-325.3261	75	-313.8165	-318.4073	-321.0013
76	-638.8145	-644.9516	-650.6354	76	-352.2080	-356.3727	-360.9716	76	-323.0236	-326.6975	-331.3637	76	-318.7569	-322.4143	-327.0129
77	-650.2367	-656.0798	-662.1503	77	-357.5379	-361.7271	-365.8760	77	-327.0844	-331.7540	-335.4094	77	-322.7719	-327.3720	-331.0120
78	-661.5315	-667.5763	-673.3450	78	-363.2725	-367.0723	-371.2462	78	-332.1221	-335.8067	-340.4843	78	-328.1629	-331.3791	-335.9871
79	-673.0949	-678.9402	-684.9159	79	-368.7554	-372.8323	-376.6066	79	-336.1794	-340.8621	-344.5289	79	-332.1832	-336.7987	-339.9864
80	0.0000	-690.5779	-696.3490	80	0.0000	-378.3335	-382.3921	80	0.0000	-344.9114	-349.6022	80	0.0000	-340.8114	-345.4346

49 nuevo resultado CBR

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Conclusiones y agradecimientos

- Son resultados preliminares de datos de problemas de optimización global similares a el problema de clústeres globales de Lennard Jones y Morse.
- Se han verificado satisfactoriamente.
- UAM-Azcapotzalco, Área de investigación: Álgebra, Geometría y Computación Científica.

¿Preguntas?