Counting free polycubes September 2024

References:

[1] W.F.Lunnon: Symmetry of cubical and general polyominoes, pp. 101-108 of R. C. Read, editor, Graph Theory and Computing. Academic Press, NY, 1972

[2] J.Mason: Coordinate sets of examples of polycube symmetry (https://oeis.org/A038119/a038119.pdf)

[3] George Sicherman: http://www.recmath.org/PolyCur/csym/

The scope of the activity was to increase the maximum term of the sequence of free polycubes to size 22, with a by-product of achieving the same goal for several related sequences.

Before this activity started, the following were the principal sequences related to polycubes:

Sequence	Description	Index of maximum term
A000162	One-sided polycubes	22
A001931	Fixed polycubes	22
A007743	Achiral polycubes	16
A038119	Free polycubes	16
A066273	Number of polycubes with n cells and rotational symmetry group of order exactly 3	14
A066281	Number of polycubes with n cells and rotational symmetry group of order exactly 4	14
A066283	Number of polycubes with n cells and rotational symmetry group of order exactly 6	14
A066287	Number of polycubes with n cells and rotational symmetry group of order exactly 8	14
A066288	Number of polycubes with n cells and rotational symmetry group of order exactly 24	14
A066453	Number of polycubes with n cells and trivial rotational symmetry group	13
A066454	Number of polycubes with n cells and rotational symmetry group of order exactly 2	13
A371397	Chiral polycubes	16

Table 1: OEIS sequences

Notes:

1. There are also polycubes with rotational symmetry group of order exactly 12, but no sequence is defined as so few terms are known.
2. [1] refers to an order of symmetry that includes both rotation and reflection, which, for achiral polycubes is twice the order of rotational symmetry referred to in the above A066xxx sequences.

The scope can be achieved, given that the numbers relative to Fixed and One-sided polycubes are known through to size 22[1], by calculating the number of polycubes of the non-trivial symmetries described in [1].

[1] Calculated by Phillip Thompson using an algorithm of Stanley Dodds

In [1], Lunnon first defines 9 geometrical operations[2] that may be performed on a polycube. These are[3]:

A: 90-degree rotation about an axis parallel to an edge of a cube.
B: 180-degree rotation about an axis parallel to an edge of a cube.
C: 180-degree rotation about an axis parallel to the diagonal of some face of a cube.
D: 180-degree rotation about an axis passing through the most distant vertices of a cube.
E: reflection in a plane parallel to a face of a cube.
F: reflection in a plane that passes through two of the most distant edges of a cube.
H: operation D followed by operation K.
J: operation A followed by operation E.
K: reflection in the centre point of the polycube.

[2] I ignore here the I operation, simple translation.
[3] I have used slightly different wording; see [1] for Lunnon's original text.

He then defines 33 symmetry classes (asymmetry + 32 symmetries) according to the following table. For example, a polycube has symmetry class BC if subjecting it to operation B yields the same polycube in precisely one way, and subjecting it to operation C yields the same polycube in precisely two ways.

	A	B	C	D	E	F	H	J	K
I	0	0	0	0	0	0	0	0	0
A	2	1	0	0	0	0	0	0	0
B	0	1	0	0	0	0	0	0	0
C	0	0	1	0	0	0	0	0	0
D	0	0	0	2	0	0	0	0	0
E	0	0	0	0	1	0	0	0	0
F	0	0	0	0	0	1	0	0	0
H	0	0	0	2	0	0	2	0	1
J	0	1	0	0	0	0	0	2	0
K	0	0	0	0	0	0	0	0	1
BB	0	3	0	0	0	0	0	0	0
BC	0	1	2	0	0	0	0	0	0
BE	0	1	0	0	1	0	0	0	1
BF	0	1	0	0	0	2	0	0	0
CE	0	0	1	0	1	1	0	0	0
CK	0	0	1	0	0	1	0	0	1
EE	0	1	0	0	2	0	0	0	0
CD	0	0	3	2	0	0	0	0	0
FF	0	0	0	2	0	3	0	0	0
AB	2	3	2	0	0	0	0	0	0
AE	2	1	0	0	1	0	0	2	1
BFF	0	3	0	0	0	2	0	2	0
CJ	0	1	2	0	2	0	0	2	0
EEE	0	3	0	0	3	0	0	0	1
EF	2	1	0	0	2	2	0	0	0
EFF	0	1	2	0	1	2	0	0	1
BD	0	3	0	8	0	0	0	0	0
CF	0	0	3	2	0	3	2	0	1
BBC	2	3	2	0	3	2	0	2	1
CCC	0	3	0	8	0	6	0	6	0
DEE	0	3	0	8	3	0	8	0	1
R	6	3	6	8	0	0	0	0	0
G	6	3	6	8	3	6	8	6	1

Table 2: Symmetry classes

For examples of each class, see [1], [2] and [3].

See Table 3 for the order of symmetry of each class.

	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32
Name	**I**	**A**	**B**	**C**	**D**	**E**	**F**	**H**	**J**	**K**	**BB**	**BC**	**BE**	**BF**	**CE**	**CK**	**EE**	**CD**	**FF**	**AB**	**AE**	**BFF**	**CJ**	**EEE**	**EF**	**EFF**	**BD**	**CF**	**BBC**	**CCC**	**DEE**	**R**	**G**
Order of symmetry	1	4	2	2	3	2	2	6	4	2	4	4	4	4	4	4	4	6	6	8	8	8	8	8	8	8	12	12	16	24	24	24	48
Order of rotational symmetry	1	4	2	2	3	1	1	3	2	1	4	4	2	2	2	2	2	6	3	8	4	4	4	4	4	4	12	6	8	12	12	24	24
Chirality	C	C	C	C	C	A	A	A	A	A	C	C	A	A	A	A	A	C	A	C	A	A	A	A	A	A	C	A	A	A	A	C	A
Contribution to fixed	48	12	24	24	16	24	24	8	12	24	12	12	12	12	12	12	12	8	8	6	6	6	6	6	6	6	4	4	3	2	2	2	1
First size	5	12	6	4	7	4	5	12	10	6	10	10	4	6	3	6	4	10	4	16	8	8	6	6	6	7	34	6	2	20	25	56	1

Table 3: Orders of symmetry

Name and order of symmetry – see [1].

Order of rotational symmetry – as used in some OEIS sequences with A066xxx numbers.

Chirality – A: Achiral, C: Chiral.

Contribution to fixed: each polycube may be oriented in this number of distinct ways and so contribute to the count of fixed polycubes. Note that contribution = 48 / order of symmetry.

First size: size of first known polycube having a specific symmetry class. See also [2].

Some formulae:

1. One-sided(n) = 2*Chiral(n) + Achiral(n)
2. Free(n) = Chiral(n) + Achiral(n)

Therefore:

3. Free(n) = (One-sided(n) + Achiral(n)) / 2

Further, consider the naming convention used in [1]. We have I for asymmetry, and the A, B, C, D, E, F, H, J, K, BB, BC, BE, BF, CE, CK, EE, CD, FF, AB, AE, BFF, CJ, EEE, EF, EFF, BD, CF, BBC, CCC, DEE, R, G for the 32 non-trivial symmetries. Say then that the number of asymmetrical polycubes of size n is Asym(n), and the number of polycubes of a specific symmetry is $Sym_i(n)$ for some i between 1 and 32.

Let $Mult_i$ be the contribution that $Sym_i(n)$ makes to Fixed(n).

4. Fixed(n) = 48 * Asym(n) + ∑ ($Mult_i$ * $Sym_i(n)$), for i = 1 to 32
5. Free(n) = Asym(n) + ∑ $Sym_i(n)$, for i = 1 to 32

Therefore, combining formulae 4 and 5, and eliminating Asym(n), we have:

6. Free(n) = (∑ ((48 - $Mult_i$) * $Sym_i(n)$) + Fixed(n)) / 48

Given that One-sided(n) is known to term 22, the quickest way to calculate Free(n) is to count the achiral polycubes[4] through to size 22 and use Formula 3.

With a reasonable extra effort, though, it is possible to calculate the numbers for the chiral polycubes with at least one rotational symmetry, and so use Formula 6 to cross-check the result of Formula 3. The division by 48 in Formula 6 raises further the confidence in the result; many errors in $Sym_i(n)$ would cause this division to fail.

Other sequences refer to polycubes with specific orders of rotational symmetry:

Sequence	Order	Formula
A066273	3	2*D(n)+H(n)+FF(n)
A066281	4	2*A(n)+2*BB(n)+2*BC(n)+AE(n)+BFF(n)+CJ(n)+EEE(n)+EF(n)+EFF(n)
A066283	6	2*CD(n)+CF(n)
A066287	8	2*AB(n)+BBC(n)
A066288	24	2*R(n)+G(n)
A066453	1	2*I(n)+E(n)+F(n)+K(n)
A066454	2	2*B(n)+2*C(n)+J(n)+BE(n)+BF(n)+CE(n)+CK(n)+EE(n)
	12	2*BD(n)+CCC(n)+DEE(n),

Table 4: Other formulae

The “missing” sequence referring to order 12 has initial values: 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 1, 1, 0.

[4] At size 16, there are about 800 times more chiral polycubes that achiral ones, so the choice of counting the latter over the former has an obvious answer.

	A	B	C	D	E	F	H	J	K	BB	BC	BE	BF	CE	CK	EE	CD	FF	AB	AE	BFF	CJ	EEE	EF	EFF	BD	CF	BBC	CCC	DEE	R	G
1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0
3	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0
4	0	0	1	0	1	0	0	0	0	0	0	1	0	0	0	1	0	1	0	0	0	0	0	0	0	0	0	2	0	0	0	0
5	0	0	2	0	6	3	0	0	0	0	0	1	0	3	0	2	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0
6	0	3	5	0	28	6	0	0	1	0	0	5	1	4	2	6	0	0	0	0	0	1	1	1	0	0	1	1	0	0	0	0
7	0	4	17	1	126	26	0	0	1	0	0	5	0	12	1	11	0	2	0	0	0	1	2	1	1	0	0	1	0	0	0	1
8	0	37	49	0	520	72	0	0	20	0	0	21	2	13	6	32	0	0	0	1	1	2	3	2	2	0	0	2	0	0	0	1
9	0	52	138	1	2099	241	0	0	17	0	0	26	2	48	5	61	0	1	0	0	0	3	4	3	1	0	0	4	0	0	0	0
10	0	342	374	9	8429	623	0	1	192	1	1	93	12	61	26	158	1	6	0	0	0	5	7	6	2	0	0	2	0	0	0	0
11	0	502	1062	1	33676	2028	0	1	175	1	2	116	9	186	17	308	0	2	0	0	0	6	12	7	4	0	0	5	0	0	0	0
12	2	2836	2851	7	135201	5374	1	6	1632	5	7	392	37	231	69	749	1	3	0	3	4	11	16	13	9	0	3	7	0	0	0	0
13	0	4343	8010	68	543248	16781	0	3	1522	3	5	497	32	727	50	1481	0	15	0	2	1	16	29	20	8	0	2	8	0	0	0	1
14	2	22622	21432	9	2195182	45094	1	10	13088	13	17	1616	134	941	235	3481	1	6	0	0	1	25	39	32	13	0	2	5	0	0	0	0
15	2	35405	60142	61	8893547	138971	0	12	12339	16	23	2087	114	2855	159	6997	1	14	0	2	2	33	73	43	19	0	1	10	0	0	0	0
16	22	176176	161386	473	36196788	378196	0	63	102846	58	78	6690	426	3707	693	16086	4	46	1	15	14	56	92	71	42	0	0	15	0	0	0	0
17	14	281141	453253	81	147739046	1156028	0	41	97374	47	62	8656	375	11293	470	32692	2	22	0	9	6	81	170	109	37	0	0	20	0	0	0	0
18	31	1363112	1222110	440	605138811	3183390	10	97	803363	136	181	27493	1393	14909	2142	74114	10	48	0	0	5	118	209	162	65	0	8	12	0	0	0	1
19	41	2205171	3436564	3316	2485051070	9679303	4	124	760594	181	218	35797	1236	44955	1399	152114	5	133	0	9	9	162	405	226	78	0	4	23	0	0	0	2
20	213	10527712	9316409	614	10233284681	26929415	6	553	6274638	546	717	113728	4398	59760	6350	341410	7	66	3	57	52	263	485	363	181	0	6	36	1	0	0	1
21	182	17221126	26231463	3315	42234214910	81575661	1	401	5928747	521	591	147838	3934	180092	4086	705978	8	161	0	40	22	380	932	553	152	0	4	48	0	0	0	0
22	321	81462884	71496106	23537	174693725151	228958790	0	821	49133524	1247	1606	469824	13883	241827	19273	1573062	20	395	0	2	21	556	1095	811	298	0	1	30	1	0	0	0
23	453	134424679						1097		1729	1835	611551	12494			3273527			0	40	32	768	2166	1150	312	0		59	1	0	0	0
24	1796	632308448						4464		4698	6002	1951237	43435			7253791			14	238	167	1229	2528	1808	772	0		80	0	0	0	1

Table 5: Results for individual symmetries

Using the above formulae, it is then possible to calculate various sequences through to size 22. New values shown in bold.

Size	Free	Achiral	Chiral
1	1	1	0
2	1	1	0
3	2	2	0
4	7	6	1
5	23	17	6
6	112	58	54
7	607	191	416
8	3811	700	3111
9	25413	2515	22898
10	178083	9623	168460
11	1279537	36552	1242985
12	9371094	143761	9227333
13	69513546	564443	68949103
14	520878101	2259905	518618196
15	3934285874	9057278	3925228596
16	29915913663	36705846	29879207817
17	**228779330204**	**149046429**	**228630283775**
18	**1758309223457**	**609246350**	**1757699977107**
19	**13573319825615**	**2495727647**	**13570824097968**
20	**105192814197984**	**10267016450**	**105182547181534**
21	**818136047201932**	**42322763940**	**818093724437992**
22	**6383528588447574**	**174974139365**	**6383353614308209**

Table 6: Final results