Fast Partial-Differential Synthesis of the Matching Polynomial of C_{72-100}

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The Thesis algorithm uses partial-differential edge operators and a grammatical structure to generate and avoid expanding the Matching Polynomial. To run the algorithm efficiently, the vertexes of fullerene graphs C_{60-100} were sorted into three-dimensional sectors.

INTRODUCTION

The Matching,[1] Reference,[2] or Acyclic[3] Polynomial is the counting polynomial of nonadjacent edges of a graph as a function of isolated vertexes. Its lowest order term is the number of perfect matchings or Kekulé structures of a given π-system. Hosoya's Z index is the number of terms in a Matching Polynomial. The Z index is elegantly calculated through graph "retrosynthesis" and easily correlates the hydrogen suppressed graph of acyclic alkanes to their boiling point. The difference in the "occupied" roots of the Matching and Characteristic Polynomials provides a method of comparing the stability of different size π-systems and is called a Topological Resonance Energy (TRE). Because of recent interest in calculating the TRE of fullerenes up to C_{70},[4−8] we report the development of the Thesis algorithm to quickly calculate the Matching Polynomial of larger fullerenes using partial-differential edge operators.

In matrix terms, for a graph G the Characteristic Polynomial, $CP(G)$ or the determinant of its adjacency matrix with elements $a_{i,j}$, is a listing of all walks across the matrix without stepping twice on the same row or column. The Matching Polynomial, $MP(G)$, is a listing of all determinant walks that contain only matching steps $a_{i,j}$ and $a_{j,i}$. $MP(G)$ equals $CP(G)$ for acyclic graphs. $MP(G)$ is a subset of $CP(G)$ for cyclic graphs because the latter includes walks that explicitly list the Hamiltonian paths of the graph.

Matching off-diagonal walks are permutations of the diagonal walk since the diagonal and off-diagonal positions of an adjacency matrix can correspond to the vertexes (v_i) and edges ($e_{i,j}$) of G, respectively, as shown in Figure 1. Rosenfeld and Gutman showed that these permutations are a product of partial-differential operators on the product of diagonal elements.[9] We use partial-differential edge operators to develop Thesis as follows.

$$\begin{bmatrix} v_1 & e_{1,2} & \dots & 0 \\ e_{2,1} & v_2 & \dots & e_{2,n_{vertices}} \\ \dots & \dots & \dots & \dots \\ 0 & e_{n_{vertices},2} & \dots & v_{n_{vertices}} \end{bmatrix}$$

Figure 1. An adjacency matrix.

```
MPC60 := Module[{}, l =
{0,1,0,12,0,48,0,0,1,2,1,59,1,1,2,3,2,11,2,2,3,4,3,58,3,3,4,5,4,9,4,4,5,6,5,56,
5,5,6,7,6,8,6,6,7,19,7,55,7,7,8,9,8,17,8,8,9,10,9,9,10,11,10,15,10,10,11,13,
11,11,12,13,12,24,12,12,13,14,13,13,14,15,14,23,14,14,15,16,15,15,16,17,
16,21,16,16,17,18,17,17,18,19,18,20,18,18,19,31,19,19,20,21,20,29,20,20,
21,22,21,21,22,23,22,27,22,22,23,25,23,23,24,25,24,36,24,24,25,26,25,25,
26,27,26,35,26,26,27,28,27,27,28,29,28,33,28,28,29,30,29,29,30,31,30,32,
30,30,31,43,31,31,32,33,32,41,32,32,33,34,33,33,34,35,34,39,34,34,35,37,
35,35,36,37,36,48,36,36,37,38,37,37,38,39,38,47,38,38,39,40,39,39,40,41,
40,45,40,40,41,42,41,41,42,43,42,44,42,42,43,55,43,43,44,45,44,53,44,44,
45,46,45,45,46,47,46,51,46,46,47,49,47,47,48,49,48,48,49,50,49,49,50,51,
50,59,50,50,51,52,51,51,52,53,52,57,52,52,53,54,53,53,54,55,54,56,54,54,
55,55,56,57,56,56,57,58,57,57,58,59,58,58,59,59};
MP = Product[v[i], {i,0,59}];
Do[
  If[l[[2 i - 1]] == l[[2 i]],
    v[l[[2 i]]] = x,
    MP = MP - D[MP, v[l[[2 i-1]]], v[l[[2 i]]]]];
  Print[i, " ", TimeUsed[], " ", MemoryInUse[]],
{i,150}];
Print[MP, " ", TimeUsed[], " ", MemoryInUse[]]}
```

Figure 2. A Mathematica program to generate *MP(C_{60})*.

<u>section 1</u> paragraph 1 sentence 17 = $w_1(l_1 l_2)$	paragraph 2 sentence 18 = $w_2(l_3 l_4)$	paragraph 3 sentence 19 = $w_3(l_5 l_6)$	paragraph 4 sentence 20 = $w_4(l_7 l_8)$
<u>section 2</u> paragraph 5 sentence 21 = $w_5(l_{17} l_{18})$		paragraph 6 sentence 22 = $w_6(l_{19} l_{20})$	
<u>section 3</u> paragraph 7 sentence 23 = $w_7(l_{21} l_{22})$			

Figure 3. $(((v_1 v_2)(v_3 v_4))((v_5 v_6)(v_7 v_8)))$.

METHODS

$MP(G)$ for the trivial graph of n vertexes is the product of the diagonal elements of the adjacency matrix, eq 1. An edge operator is a permutor of the diagonal walk to its matching off-diagonal elements, eq 2. $MP(G)$ for a nontrivial graph is the product of edge operators on the trivial graph monomial as shown in eq 3. Partial-differential operators ensure that no row or column is repeated in a walk since the

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section 1			
paragraph 1	paragraph 2	paragraph 3	paragraph 4
sentence 17 = $w_1(l_1l_2)+w_8(l_9l_{10})$	sentence 18 = $w_2(l_3l_4)$	sentence 19 = $w_3(l_5l_6)$	sentence 20 = $w_4(l_7l_8)$
section 2			
paragraph 5		paragraph 6	
sentence 21 = $w_5(l_{17}l_{18})$		sentence 22 = $w_6(l_{19}l_{20})$	
section 3			
paragraph 7			
sentence 23 = $w_7(l_{21}l_{22})$			

Figure 4. $((E_{1,2}(v_1v_2)(v_3v_4))((v_5v_6)(v_7v_8)))$.

section 1			
paragraph 1	paragraph 2	paragraph 3	paragraph 4
sentence 17 = $w_1(l_1l_2)+w_8(l_9l_{10})$	sentence 18 = $w_2(l_3l_4)$	sentence 19 = $w_3(l_5l_6)$	sentence 20 = $w_4(l_7l_8)$
sentence 24 = $w_9(l_1l_{10})$	sentences 25 = $w_{10}(l_{11}l_4)$		
section 2			
paragraph 5		paragraph 6	
sentence 21 = $w_5(l_{17}l_{18})+w_{11}(l_{24}l_{25})$		sentence 22 = $w_6(l_{19}l_{20})$	
section 3			
paragraph 7			
sentence 23 = $w_7(l_{21}l_{22})$			

Figure 5. $(E_{2,3}(E_{1,2}(v_1v_2)(v_3v_4))((v_5v_6)(v_7v_8)))$.

section 1			
paragraph 1	paragraph 2	paragraph 3	paragraph 4
sentence 17 = $w_1(l_1l_2)+w_8(l_9l_{10})$	sentence 18 = $w_2(l_3l_4)+w_{12}(l_{11}l_{12})$	sentence 19 = $w_3(l_5l_6)+w_{20}(l_{13}l_{14})$	sentence 20 = $w_4(l_7l_8)+w_{26}(l_{15}l_{16})$
sentence 24 = $w_9(l_1l_{10})$	sentence 25 = $w_{10}(l_{11}l_4)$	sentence 28 = $w_{15}(l_{13}l_6)$	sentence 33 = $w_{23}(l_{15}l_8)$
	sentence 26 = $w_{13}(l_3l_{12})$	sentence 31 = $w_{21}(l_5l_{14})$	
	sentence 27 = $w_{14}(l_{11}l_{12})$	sentence 32 = $w_{22}(l_{13}l_{14})$	
section 2			
paragraph 5		paragraph 6	
sentence 21 = $w_5(l_{17}l_{18})+w_{11}(l_{24}l_{25})$		sentence 22 = $w_6(l_{19}l_{20})+w_{24}(l_{31}l_{33})$	
sentence 29 = $w_{16}(l_{17}l_{26})+w_{17}(l_{14}l_{27})$		sentence 30 = $w_{18}(l_{28}l_{20})+w_{25}(l_{32}l_{33})$	
section 3			
paragraph 7			
sentence 23 = $w_7(l_{21}l_{22})+w_{19}(l_{29}l_{30})$			

Figure 6. $E_{4,5}(E_{2,3}(E_{1,2}(v_1v_2)E_{3,4}(v_3v_4))E_{6,7}(E_{5,6}(v_5v_6)E_{7,8}(v_7v_8)))$.

last term of eq 4 cancels on a monomial with all terms to the first power.

$$MP(G_{trivial}) = \prod_{i=1}^{n_{vertices}} v_i \tag{1}$$

$$E_{j,k}^{-} = 1 - \frac{e_{j,k}e_{,k,j}\partial^2}{\partial v_j \partial v_k} \tag{2}$$

$$MP(G) = \prod_{m=1}^{n_{edges}} E_{j,k(m)}^{-} \prod_{i=1}^{n_{vertices}} v_i \tag{3}$$

$$E_{j,k}^{-}E_{j,l}^{-} = 1 - \frac{e_{j,k}e_{k,j}\partial^2}{\partial v_j \partial v_k} - \frac{e_{j,l}e_{l,j}\partial^2}{\partial v_j \partial v_l} + \frac{e_{j,k}e_{k,j}e_{j,l}e_{l,j}\partial^4}{(\partial v_j)^2 \partial v_k \partial v_l} \tag{4}$$

The positive edge operator shown in eq 5 generates *$MP^+(G)$*, the permanental equivalent of *MP(G)*, or allows

Table 1. Matching Polynomials

C_n, axis	60y	70z
$MP^+(C_n)$ time/s	7	23
Letters/Sentences	5497	7777
Words	68026	143319
$MP^+(C_n,1)$ time/s	0	0
Z index	1.417036634543488E+15	4.760609105256725E+17
$MP^+(C_n, x)$ time/s	36	147
Order	Coefficients	
x^0	12500	52168
x^2	4202760	24949770
x^4	269272620	2175411410
x^6	6946574300	76188054720
x^8	94541532165	1414031839415
x^{10}	783047312406	16060741380337
x^{12}	4310718227685	121977585926655
x^{14}	16742486291340	657705883833585
x^{16}	47883826976580	2.62862680607528E+15
x^{18}	104113567937140	8.04243921720919E+15
x^{20}	176345540119296	1.93119181605115E+16
x^{22}	237135867688980	3.71169893763219E+16
x^{24}	256967614454320	5.80047715746414E+16
x^{26}	227043126274260	7.46502399971658E+16
x^{28}	165074851632300	7.99431035976412E+16
x^{30}	99463457244844	7.18431674843235E+16
x^{32}	49924889888850	5.45534213776560E+16
x^{34}	20949286202160	3.51942821425224E+16
x^{36}	7362904561730	1.93727575573052E+16
x^{38}	2168137517940	9.12760379418898E+15
x^{40}	534162544380	3.68887741125418E+15
x^{42}	109742831260	1.28023674340454E+15
x^{44}	18697786680	381580564799125
x^{46}	2619980460	97578536447295
x^{48}	298317860	21362502290720
x^{50}	27130596	3989784929340
x^{52}	1922040	632435470975
x^{54}	102120	84479881155
x^{56}	3825	9417493125
x^{58}	90	864583005
x^{60}	1	64182939
x^{62}		3753855
x^{64}		166390
x^{66}		5250
x^{68}		105
x^{70}		1

graph-polynomial degradation since conjugate edge operators annihilate each other, eq 6. The coefficients of *$MP^+(G)$* are identical to those of *MP(G)* except for the alternating sign of the latter.

$$E_{j,k}^{+} = 1 + \frac{e_{j,k}e_{k,j}\partial^2}{\partial v_j \partial v_k} \tag{5}$$

$$E_{j,k}^{+}E_{j,k}^{-} = 1 \tag{6}$$

Though easily calculated in a symbolic language, an expanded multivariable *$MP(C_n)$* of a fullerene is too large to represent as indicated by a huge Z index. For example, the Mathematica 3.0 program given in Figure 2 uses 64 MB of RAM to generate *$MP(C_{60}, x)^{10}$* ($Z = 1.4 \times 10^{15}$) in 31 min on a 200 MHz PC even as it substitutes each variable v[i] with x after it applies all three partial differentials with respect to v[i]. The edge operator is simply MP = MP − D[MP, v[j], v[k]].

Table 2. Matching Polynomials

C_n, axis	72z	74x	76y	78y	80y
$MP^+(C_n)$ time/s	11	68	141	296	67
Letters/Sentences	6449	11965	13145	19729	14049
Words	85430	295299	269203	524504	251827
$MP^+(C_n,1)$ time/s	0	0	0	2	1
Z index	1.52379191124229E+18	4.87723412503989E+18	1.56111894462469E+19	4.99675838961259E+19	1.59939535739180E+20
$MP^+(C_n, x)$ time/s	88	358	392	1162	473
Order	Coefficients				
x^0	77400	85119	124439	156492	270153
x^2	37159200	48987655	72619922	98800572	154287610
x^4	3345162432	4848711174	7412804855	10828448538	16929185015
x^6	122558197024	190727707272	304216122936	472462895226	759118423260
x^8	2393469043524	3967349630137	6638334607776	10914789369489	18226025554255
x^{10}	28704598608024	50517449105277	88961463590540	154590472784429	269901774808282
x^{12}	230726853211188	430627522112217	799856605022370	1.46823749361833E+15	2.69001312432190E+15
x^{14}	1.31898643509007E+15	2.61035469851254E+15	5.12225664595390E+15	9.93360222158052E+15	1.91446844802899E+16
x^{16}	5.59699938864125E+15	1.17504201292631E+16	2.43915637670210E+16	4.99989809654693E+16	1.01539980138955E+17
x^{18}	1.82054495202396E+16	4.05752309655063E+16	8.92040273492884E+16	1.93415315887395E+17	4.14469553608037E+17
x^{20}	4.65353337781300E+16	1.10208471787750E+17	2.56903055033695E+17	5.89701006528408E+17	1.33497041515992E+18
x^{22}	9.53335342177769E+16	2.40174529397287E+17	5.94308732175795E+17	1.44560744016319E+18	3.46105893588590E+18
x^{24}	1.59022409077892E+17	4.26699556232873E+17	1.12217782055981E+18	2.89559777335120E+18	7.33997315468986E+18
x^{26}	2.18777389029217E+17	6.26092843822986E+17	1.75223264349507E+18	4.80189419050786E+18	1.29021415505063E+19
x^{28}	2.50867862188707E+17	7.66838416655156E+17	2.28704925036547E+18	6.66489204511052E+18	1.90046627743091E+19
x^{30}	2.41841995535982E+17	7.90915835864830E+17	2.51756612528356E+18	7.81266999633002E+18	2.36727475701722E+19
x^{32}	1.97390379486861E+17	6.91922917615568E+17	2.35457445507588E+18	7.79281910386050E+18	2.51268698222238E+19
x^{34}	1.37186081385089E+17	5.16483035441874E+17	1.88241461447674E+18	6.65564432794572E+18	2.28716588195066E+19
x^{36}	8.15562824476536E+16	3.30521919926091E+17	1.29286051251143E+18	4.89242772379036E+18	1.79486023740923E+19
x^{38}	4.16182217459096E+16	1.82022053785676E+17	7.65872706801153E+17	3.10828112740624E+18	1.21965205251733E+19
x^{40}	1.82758931121746E+16	8.65080134048396E+16	3.92534022065706E+17	1.71248417438422E+18	7.20194976876803E+18
x^{42}	6.91711944853812E+15	3.55503610480707E+16	1.74461384797952E+17	8.20251581169898E+17	3.70576975589466E+18
x^{44}	2.25788287473569E+15	1.26462258771376E+16	6.73380655755124E+16	3.42183136543101E+17	1.66500700747724E+18
x^{46}	635430812245836	3.89497654463288E+15	2.25868113853741E+16	1.24456872952675E+17	6.54123061107341E+17
x^{48}	153971990229848	1.03795974550506E+15	6.58299169898385E+15	3.94788845138592E+16	2.24858643016567E+17
x^{50}	32043716476716	238927993751013	1.66545778990140E+15	1.09169335400248E+16	6.76341876476514E+16
x^{52}	5705866140966	47376763450332	365043553466658	2.62829224777568E+15	1.77874245071628E+16
x^{54}	864652893884	8059708499592	69111636139668	549713259720419	4.08404773674106E+15
x^{56}	110690579973	1169765435812	11253888461463	99560855449381	816690124439395
x^{58}	11852752392	143756363544	1567057426890	15545196957717	141751784201960
x^{60}	1047459326	14808816255	185159638887	2080030465219	21256630567074
x^{62}	74997996	1261482041	18375347268	236640822375	2737145542380
x^{64}	4238379	87223566	1510756122	22653950949	300233075775
x^{66}	181836	4768338	100993272	1799779445	27759330840
x^{68}	5562	198209	5346486	116448918	2133467090
x^{70}	108	5883	215536	5975658	133740732
x^{72}	1	111	6213	233844	6658770
x^{74}		1	114	6552	253160
x^{76}			1	117	6900
x^{78}				1	120
x^{80}					1

We developed Thesis to avoid full expansion of MP(G) and to make its calculation portable to other applications. We illustrate how Thesis works by calculating *MP(G)* for an eight-vertex chain, G_8. The general concept is to first associate the vertex variables v_{1-8} into binary groups. Then apply edge operators only to those groups to which they pertain without expanding the polynomial, eq 7.

$$MP(G_8) = E_{4,5}(E_{2,3}(E_{1,2}(v_1v_2)E_{3,4}(v_3v_4))E_{6,7}(E_{5,6}(v_5v_6)E_{7,8}(v_7v_8))) \quad (7)$$

To program these parenthetic associations we call the product of two letters a word, the summation of words a sentence, a collection of sentences with the same pair of letters and their derivatives a paragraph, and a collection of paragraphs representing the same power of two vertex variables a section. For the trivial graph of our eight-vertex example the vertex variables v_{1-8} are letters and sentences one through eight because the sentences of one section are the letters of the next. We reserve letters and sentences 9−16 as the partial derivative of each vertex variable. The product of all vertex variables is sentence 23 in Figure 3.

To apply edge operators we follow two simple rules. The first is that we add words corresponding to the partial derivative of existing words to existing sentences if both letters in a section are in the same paragraph. Figure 4 illustrates applying $E_{1,2}$.

The second rule is to create new sentences corresponding to the partial derivative of existing sentences if both letters

Table 3. Matching Polynomials

C_n, axis	82y	84z	86z	88y	90z
$MP^+(C_n)$ time/s	187	177	90	182	73
Letters/Sentences	22001	22937	19713	27025	14365
Words	572968	461144	369670	510283	359071
$MP^+(C_n, 1)$ time/s	1	0	0	0	0
Z index	5.11928718764056E+20	1.63856268904723E+21	5.24468210787329E+21	1.67872807888161E+22	5.37323821892860E+22
$MP^+(C_n, x)$ time/s	1358	1017	517	655	830
Order	Coefficients				
x^0	320678	379824	490858	688905	917357
x^2	210425094	284664296	397470352	581610216	802577425
x^4	24719893280	35894363486	52774304177	79570986926	115893854312
x^6	1173402008208	1804293964056	2785793083095	4355866266252	6666679806262
x^8	29712524748568	48164593645498	78037042251960	127062169844979	203903751995185
x^{10}	463448764669230	790639953232716	1.34413806102803E+15	2.28504416081282E+15	3.84169239203539E+15
x^{12}	4.86373029527818E+15	8.72780073849130E+15	1.55729862035761E+16	2.76914326099719E+16	4.87676903569649E+16
x^{14}	3.64559939565595E+16	6.88155699555264E+16	1.28929546125292E+17	2.40123014120335E+17	4.43069887420676E+17
x^{16}	2.03737774867215E+17	4.04702551475871E+17	7.96618191509479E+17	1.55563942273589E+18	3.00869360045485E+18
x^{18}	8.76845770543761E+17	1.83392481782712E+18	3.79515735534971E+18	7.77807263579532E+18	1.57762141832013E+19
x^{20}	2.98009884415206E+18	6.56726345676912E+18	1.42981367300995E+19	3.07807997257116E+19	6.55147257414098E+19
x^{22}	8.15957254803518E+18	1.89608693707620E+19	4.34647369383287E+19	9.83693203379671E+19	2.19857044161147E+20
x^{24}	1.82918480908978E+19	4.48602002019312E+19	1.08364013081853E+20	2.58045605331435E+20	6.06060508782894E+20
x^{26}	3.40227353430684E+19	8.81442556489712E+19	2.24569112643115E+20	5.63156235941557E+20	1.39100100749122E+21
x^{28}	5.30869929389258E+19	1.45437481845893E+20	3.91183045112590E+20	1.03400878090614E+21	2.68822867314760E+21
x^{30}	7.01316157441734E+19	2.03396987380561E+20	5.78153600929652E+20	1.61240987976462E+21	4.41622872643574E+21
x^{32}	7.90501891143040E+19	2.42994161750870E+20	7.30756707871511E+20	2.15251240494216E+21	6.21692576062387E+21
x^{34}	7.65200222345155E+19	2.49629473394701E+20	7.95197004806551E+20	2.47671332145536E+21	7.55112982066070E+21
x^{36}	6.39577211045978E+19	2.21747601185694E+20	7.49219512117075E+20	2.47039137997493E+21	7.95970234368375E+21
x^{38}	4.63683829028445E+19	1.71123290710403E+20	6.14117825180271E+20	2.14653095134113E+21	7.31800531171013E+21
x^{40}	2.92667765791499E+19	1.15166518726371E+20	4.39684560417568E+20	1.63147448330493E+21	5.89299569062308E+21
x^{42}	1.61303991208751E+19	6.78078750982010E+19	2.75876347226549E+20	1.08840579398274E+21	4.17133289046894E+21
x^{44}	7.78089199358390E+18	3.50151176201921E+19	1.52101276287691E+20	6.39141877487515E+20	2.60313329344390E+21
x^{46}	3.29035331597129E+18	1.58879973003045E+19	7.38415823931041E+19	3.31116513537734E+20	1.43565220830645E+21
x^{48}	1.22102414742388E+18	6.34276887905031E+18	3.16139436455166E+19	1.51596584427240E+20	7.01064499801874E+20
x^{50}	3.97775791447798E+17	2.22939634041631E+18	1.19477670568923E+19	6.14109199149597E+19	3.03552155185174E+20
x^{52}	1.13727112935867E+17	6.89981516429734E+17	3.98755772544341E+18	2.20267030511790E+19	1.16647956588782E+20
x^{54}	2.85087478249248E+16	1.87932496409059E+17	1.17510242341165E+18	6.99642307971085E+18	3.97999653381438E+19
x^{56}	6.25499399060569E+15	4.49948363695267E+16	3.05541770811986E+17	1.96728254236543E+18	1.20567435461425E+19
x^{58}	1.19807405290313E+15	9.45108082362743E+15	6.99985583315508E+16	4.89231564857801E+17	3.24097610567293E+18
x^{60}	199613017530388	1.73682473394837E+15	1.40999347832669E+16	1.07433794547125E+17	7.72213075257761E+17
x^{62}	28791516388176	278200981687320	2.48991334737386E+15	2.07856573294394E+16	1.62804870131447E+17
x^{64}	3572666166791	38650064176962	383973726246580	3.53224757981357E+15	3.02986074543787E+16
x^{66}	378300437241	4627612461276	51448668624636	525119833781136	4.96152726323661E+15
x^{68}	33820515738	473579561586	5950836847628	67942315851528	711951401910385
x^{70}	2517176370	40982161284	589225290720	7600232587048	89050481340507
x^{72}	153027609	2956732589	49405928097	728860281702	9644087121125
x^{74}	7398819	174477354	3458455529	59271938640	896628926415
x^{76}	273511	8198883	198266925	4029186666	70780315005
x^{78}	7257	294924	9062121	224582676	4676317115
x^{80}	123	7623	317426	9991773	253620600
x^{82}	1	126	7998	341044	10991160
x^{84}		1	129	8382	365805
x^{86}			1	132	8775
x^{88}				1	135
x^{90}					1

in a section are not in the same paragraph. These new sentences are the partial derivatives of letters in the next section as shown by applying $E_{1,2}$ and $E_{2,3}$ in Figure 5.

We apply the second rule from section to section until both letters in a section are in the same paragraph and rule one applies. For example, $E_{4,5}$ applies up to section 3. We illustrate this and the other operators required to complete the eight-vertex chain polynomial in Figure 6. The words show the trail of operations.

To calculate $MP^+(G, x)$ we substitute the same variable for letters one through eight, substitute one into partial derivative letters 9−16, and evaluate Thesis up to the only sentence of the last section, sentence 23. To calculate MP-(G, x) we substitute complex i into letters 9−16.

A measure of the efficiency of Thesis is the multiplications and additions it performs. For Thesis they both equal the number of words. To minimize this number we must apply the edge operators within the smallest parenthetic association. Since this is similar to numbering vertexes by spatial proximity, we sorted the n vertexes of the graph of fullerenes C_{60-100} into $n/2$ sectors around the x, y or z axis using the three-dimensional coordinates from Mitsuho Yoshida's Fullerene Gallery.[11] The axis was chosen for maximum total interconnectivity between sectors.

Table 4. Matching Polynomials

C_n	92y	94x	96z	98z	100z
$MP^+(C_n)$ time/s	1186	1307	1938	794	568
Letters/Sentences	35769	42353	44353	37973	38281
Words	1122018	1456529	1575102	1276492	1042116
$MP^+(C_n, 1)$ time/s	1	2	5	2	2
Z index	1.71985828794839E+23	5.50494020206795E+23	1.76202706697029E+24	5.63989823822308E+24	1.80522986774562E+25
$MP^+(C_n, x)$ time/s	1596	2461	2407	1903	1690
Order	Coefficients				
x^0	1227892	1717113	2484405	3449999	4860048
x^2	1128529824	1629491064	2361300848	3366974673	4923127152
x^4	170081741686	253639287154	378315347620	558695871968	837774868148
x^6	10220043039970	15801570660777	24397056014732	37397269080004	57806823762648
x^8	326677451854290	525114082464828	841814374079479	1.34132449044513E+15	2.14501534830138E+15
x^{10}	6.43450771472702E+15	1.07734686901909E+16	1.79682726626372E+16	2.97936219378285E+16	4.94152151461148E+16
x^{12}	8.54258216496516E+16	1.49185646799072E+17	2.59226949307615E+17	4.47702860963233E+17	7.71511484873870E+17
x^{14}	8.12060293108491E+17	1.48075416393348E+18	2.68354198007144E+18	4.83111385202231E+18	8.66148153544896E+18
x^{16}	5.77264441142331E+18	1.10003932561742E+19	2.08109133591915E+19	3.90805806564196E+19	7.29710142895563E+19
x^{18}	3.17048152485141E+19	6.31881923709455E+19	1.24885762143870E+20	2.44791438970175E+20	4.76435524429732E+20
x^{20}	1.37991399605296E+20	2.87843712322073E+20	5.94755693644695E+20	1.21761206770366E+21	2.47208103835503E+21
x^{22}	4.85655299065704E+20	1.06104978367757E+21	2.29362456955075E+21	4.90740578654168E+21	1.04004696548025E+22
x^{24}	1.40501571622822E+21	3.21737916499875E+21	7.28102240096875E+21	1.62913745877554E+22	3.60657839937090E+22
x^{26}	3.38682325255968E+21	8.13478300460710E+21	1.92861023801451E+22	4.51575503936113E+22	1.04494115608472E+23
x^{28}	6.87978507893075E+21	1.73457536177522E+22	4.31137746779445E+22	1.05710760484147E+23	2.55856313735979E+23
x^{30}	1.18896994876670E+22	3.14922919968494E+22	8.21264166012606E+22	2.11015749714758E+23	5.34574907135504E+23
x^{32}	1.76237683692149E+22	4.90816268804828E+22	1.34401331667806E+23	3.62154382265639E+23	9.60990501137653E+23
x^{34}	2.25611390769231E+22	6.61248472935867E+22	1.90295222731655E+23	5.38178117256176E+23	1.49697642696824E+24
x^{36}	2.50915052305948E+22	7.74710001969281E+22	2.34519569002197E+23	6.96720031276588E+23	2.03311927324229E+24
x^{38}	2.43665920181069E+22	7.93366241855152E+22	2.52881758404502E+23	7.89909080469775E+23	2.42031841857407E+24
x^{40}	2.07511827998723E+22	7.13316820199714E+22	2.39656898168971E+23	7.87877550960850E+23	2.53715148750139E+24
x^{42}	1.55548202026271E+22	5.65197993459977E+22	2.00386436748495E+23	6.94077715369203E+23	2.35135920404032E+24
x^{44}	1.02943979779493E+22	3.95926186766457E+22	1.48313274354461E+23	5.41863064043606E+23	1.93324827716773E+24
x^{46}	6.03056961347605E+21	2.45857358563025E+22	9.74386783423532E+22	3.75967985959024E+23	1.41428582960083E+24
x^{48}	3.13349495139676E+21	1.35630895831984E+22	5.69542136532706E+22	2.32403184150999E+23	9.22909654502461E+23
x^{50}	1.44644007174719E+21	6.65878915832877E+21	2.96740961217629E+22	1.28241825465468E+23	5.38352549352242E+23
x^{52}	5.93830719006832E+20	2.91313025858076E+21	1.38013133399015E+22	6.32713581953383E+22	2.81193901987346E+23
x^{54}	2.16975488816662E+20	1.13667345384530E+21	5.73607209081543E+21	2.79448521756669E+22	1.31693173656190E+23
x^{56}	7.05736866264567E+19	3.95751676499548E+20	2.13180880354649E+21	1.10580539906937E+22	5.53568386512271E+22
x^{58}	2.04293387026751E+19	1.22951707510270E+20	7.08657885859432E+20	3.92230371455485E+21	2.08982627622981E+22
x^{60}	5.25927564949173E+18	3.40714318966786E+19	2.10677046503333E+20	1.24717839171592E+21	7.08773271435867E+21
x^{62}	1.20255903901998E+18	8.41400206949402E+18	5.59810336437890E+19	3.55393813741785E+20	2.15940202262696E+21
x^{64}	2.43774061505819E+17	1.84909099661523E+18	1.32818431864072E+19	9.06930850602106E+19	5.90739466109798E+20
x^{66}	4.36988004462340E+16	3.60905337957877E+17	2.80931641260828E+18	2.07021864302448E+19	1.44986610644174E+20
x^{68}	6.90421377332259E+15	6.23960777221982E+16	5.28631429200341E+17	4.22003737108403E+18	3.18840209352821E+19
x^{70}	957371180909612	9.52282543471302E+15	8.82508098921638E+16	7.66501979189399E+17	6.27141495365482E+18
x^{72}	115886941689630	1.27742518182741E+15	1.30248038810988E+16	1.23699596922613E+17	1.10078322464784E+18
x^{74}	12162592853488	149793959786451	1.69195341140560E+15	1.76732329327589E+16	1.71911236871639E+17
x^{76}	1097255803434	15249528727410	192381342354918	2.22535284735764E+15	2.37997324239688E+16
x^{78}	84152799804	1336108909218	19014126689476	245570910359103	2.90746834723139E+15
x^{80}	5407816304	99634462353	1619267922318	23583137883942	311646966525189
x^{82}	285586572	6232261377	117495492336	1953597760854	29103114196610
x^{84}	12063684	320696592	7158867326	138033083136	2346827700075
x^{86}	391736	13212828	359177028	8197517852	161573407020
x^{88}	9177	418864	14442156	401264859	9358796955
x^{90}	138	9588	447216	15755313	447207918
x^{92}	1	141	10008	476819	17156025
x^{94}		1	144	10437	507700
x^{96}			1	147	10875
x^{98}				1	150
x^{100}					1

RESULTS AND DISCUSSION

Tables 1−4 list the coefficients of $MP^+(C_{60-100}, x)$ generated by Thesis, one example per size, on a SGI Indigo2 with R4000-150 MHz processor and 96 MB RAM. Retention of the 15-digit precision of the double data type is shown for the known coefficients of $MP^+(C_{60-70})$[6,10] in Table 1. Because this C program uses dynamic memory allocation, the times shown to generate $MP(G)$ are 10 times greater than if predefined arrays are used. In all cases it takes more time to generate $MP^+(C_n, x)$ than $MP(C_n)$. Both a PC and SGI executable along with over 1000 sector sorted fullerene files can be downloaded.[12]

The letters and sentences are the number of variables and parentheses, respectively, used to represent $MP(C_n)$ without expansion. For Thesis both are equal as given in Tables 1−4. That the growth of this number and the number of words does not correlate with the number of vertexes, whereas the growth in the coefficients of $MP^{+}(C_n, x)$ does, indicates that the numbering of the vertexes is not optimum.

Because of the evolution of computer power and increased use of RAM versus much slower virtual memory among other factors,[13] there is no direct method of comparing Thesis to other recently developed algorithms for generating $MP(C_n, x)$.[8,14] Our best estimate is that Thesis with dynamic memory allocation generates $MP^{+}(C_{70}, x)$ about as fast as the current record of 14 min for $MP(C_{70}, x)$ on a 486-66 MHz PC,[8] i.e., 2 min 14 s for $MP(C_{70})$ and 26 min 42 s for $MP^{+}(C_{70}, x)$ on our 486-33 MHz PC (16 MB RAM + virtual memory). Nevertheless edge operators simplify the synthetic concept and the algebra of calculating $MP(G)$ to give the never before published $MP^{+}(C_n, x)$ of fullerenes above C_{70}.

Since the 15-digit precision of the coefficients given in Tables 1−4 is insufficient to calculate the roots of $MP(C_n, x)$ approaching ± 3, directly using $MP(C_n)$ to calculate the roots of $MP(C_n, x)$ is our next focus. It will also be interesting to analyze $MP(C_n, x)$ along family lines.[15,16]

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