```
restart: with(LinearAlgebra): with(Optimization):
# This MAPLE file takes a list of triangulations computed in sage (via TOPCOM package) and gives as
    output a series of polynomial expressions.
# Each set of expressions f_1,...,f_m can be used to produce a region of multistationarity for the n-site
   phosphorylation system as f 1>0,...,f m>0.
# set n
n := 4:
# Since the tables are going to be big, increase the maximum allowed size for tables.
```

 $interface(rtablesize = 4 + 2 \cdot n)$ : # set T[-1] and the matrices A, C and Csimple.

T[-1] := 1:

A := Transpose(Matrix([[1, 0, 0], [0, 1, 0], [0, 0, 1], seq([1, i, -i], i = 1 ..n), seq([1, i, 1 - i], i = 1))..n), [0, 0, 0]));

 $C := Transpose(Matrix([[1, 0, 0], [0, 1, 0], [0, 0, 1], seq([T[i], 0, 0], i = 0..n - 1), seq([K[i] \cdot T[i], i = 0..n - 1)))$ -1] +  $L[i] \cdot T[i]$ ,  $K[i] \cdot T[i-1]$ ,  $L[i] \cdot T[i]$ , i = 0..n - 1), [-S, -E, -F]]));

Csimple := Transpose(Matrix([[1, 0, 0], [0, 1, 0], [0, 0, 1], seq([1, 0, 0], i = 0..n - 1), seq([1, 0], i = 0..n -M[i], 1 - M[i], i = 0..n - 1), [-S, -E, -F])

# Here we define the procedure Foundariginaltriang that we will use in the end of the present script.

# This will be used when we need to recover the triangulation in L1 that gave a element in L7 used to obtain a region of multistationarity.

```
Foundoriginal triang := proc(original, T)
local k, aux;
aux := T:
for k from 1 to numelems(original) do
if \{op(T)\}\ subset \{op(original[k][2])\}\ then aux := original[k][1]\ fi
od:
aux;
end proc:
```

# Here we define validpolytopesindex as the set of triples that index all non zero 3 x3 minors of Csimple. # This will be used to pass from L2 to L3.

```
validpolytopesindex := []:
```

```
for il from 1 to ColumnDimension(Csimple) do
for i2 from i1 + 1 to ColumnDimension (Csimple) do
for i3 from i2 + 1 to ColumnDimension (Csimple) do
if Determinant(Csimple [1..3, [i1, i2, i3]]) \neq 0 then validpolytopesindex
     := [op(validpolytopesindex), [i1, i2, i3]];
end if
end do end do end do:
# Here we import L1 from a file outputed from SAGE, this is step (1) in the Algorithm.
L1 := parse(ImportData()):
# Here we do step (2) of Algorithm to obtain L2 from L1.
# The variables "originals", "originals2",..., will keep track from the passage from L1 to L2, L2 to L3 and
    so on.
L2 := \{ \} :
# We define L2 as a empty list and look at the elements of L1 one by one.
# In each triangulation of L1 we will take only the simplices that contain the last vertex and insert those
    in L2.
# In order to pass from L2 to L3 and so on the technique will be the same, start with a empty list and
    insert the right elements from the preivous one.
# The originals list is a link between L2 and L3 used after to recover elements of L1 from L2.
originals := \{ \} :
for i from 1 to numelems(L1) do
# Here we reset the variable "auxi2" that will hold the set of simplices of the triangulation L1[i] to be
    inserted in L2.
auxi2 := [];
for l from 1 to numelems(L1[i]) do
# Here we reset the variable "auxi" that will hold (the indexes of) the simplex we are testing.
auxi := [0, 0, 0, 0];
for j from 1 to 4 do
# This line is needed because on SAGE the vertex are indexed beginning with 0 and we want that they
    start from 1.
auxi[j] := L1[i][l][j] + 1;
od:
# The next "if" makes Step (2) passing from L1 to L2 only the simplexes with the last vertex.
if auxi[4] = ColumnDimension(C) then auxi2 := [op(auxi2), auxi]; fi:
od:
# In the next line we indeed insert in L2 the set of simplices "auxi2", but only if it is not there yet.
if not(member(auxi2, L2)) then
L2 := \{op(L2), auxi2\};
originals := originals union \{ [L1[i], auxi2] \} :
fi:
od:
# Here we do step (3) of Algorithm to obtain L3 from L2
    by removing all simplices with a corresponding matrix having a zero 3 x3 minor.
# The script is pretty much the same as step (2) but with distinct test condition.
```

 $L3 := \{ \} :$ 

```
# The originals 2 list is a link between L2 and L3 used after to recover elements of L2 from L3.
originals2 := \{ \} :
for i from 1 to numelems(L2) do
auxi := [\ ];
for l from 1 to numelems(L2[i]) do
# The next "if" makes Step (3) passing from L2
    to L3 only simplexes whose corresponding matrix has no zero 3 x3 minor.
if { [L2[i][l][1], L2[i][l][2], L2[i][l][3]], [L2[i][l][1], L2[i][l][2], L2[i][l][4]], [L2[i][l][1],
    L2[i][l][3], L2[i][l][4]], [L2[i][l][2], L2[i][l][3], L2[i][l][4]]}
    subset { op(validpolytopesindex) } then
auxi := [op(auxi), L2[i][l]];
fi:
od:
if not(member(auxi, L3)) then
L3 := L3 \text{ union } \{auxi\};
originals2 := originals2  union \{ [L2[i], auxi] \} :
fi:
od:
# Here we do step (4) of Algorithm to obtain L4 from L3 changing any index 4, 5,..., n + 3 to 1.
L4 := \{ \}:
# The originals 3 list is a link between L2 and L3 used after to recover elements of L3 from L4.
originals 3 := \{ \}:
for i from 1 to numelems(L3) do
auxi := [\ ];
for l from 1 to numelems(L3[i]) do
auxi2 := L3[i][l]:
for j from 4 to n + 3 do
# The next line tests if j is a index of L3[i], if it is bb receives true and pp its position.
bb := member(j, L3[i][l], pp');
if bb = true then
auxi2[pp] := 1; \mathbf{fi}; \mathbf{od};
# After changing some index to 1 we sort the list of simplices to keep it in the lexicographic order.
auxi := sort([op(auxi), sort(auxi2)]);
od:
# The next line is need because after changing some index to we can have duplicates.
if not(member(auxi, L4)) then
L4 := L4 \text{ union } \{auxi\};
# The originals 3 list is a link between L3 and L4 used after to recover elements of L3 from L4.
originals3 := originals3  union \{[L3[i], auxi]\}:
fi:
od:
# Here we do step (5) of Algorithm to obtain L5 from L4.
L5 := \{ \} :
```

```
for i from 1 to numelems (L4) do
# If the variable "auxi" is 0 we insert L4[i] in L5, and if it is 1 we do not.
# We reset "auxi" as 0 in the next line.
auxi := 0:
# The next loop for will test if L4[i] is contained in any L4[j] with j > i, if it is then we set auxi:=1.
for j from i + 1 to numelems(L4) while auxi = 0 do
if numelems(\{op(L4[i])\}\) intersect \{op(L4[j])\}) = numelems(L4[i]) then
auxi := 1;
fi;
 od:
if auxi = 0 then
L5 := L5 \text{ union } \{L4\lceil i\rceil\}
 fi:
 od:
# The following is just a information check.
print("This list L1 is the whole list.");
print("This list L2 consider only the simplices having the origin.");
print("This list L3 takes out the simplices which the corresponding matrix has a zero 3x3 minor.");
print("This list L4 replaces indexes 4,5,...,n+3 by 1.");
    print("This list L5 takes out the triangulations T such that there is another triangulation T'
    containing T.");
print("Number of elements of L1, L2,L3, L4, and L5 are.");
nops(L1); nops(L2); nops(L3); nops(L4); nops(L5);
                                  "This list L1 is the whole list."
                   "This list L2 consider only the simplices having the origin."
   "This list L3 takes out the simplices which the corresponding matrix has a zero 3x3 minor."
                         "This list L4 replaces indexes 4,5,...,n+3 by 1."
"This list L5 takes out the triangulations T such that there is another triangulation T' containing T.
                       "Number of elements of L1, L2,L3, L4, and L5 are."
                                               9094
                                               2728
                                                682
                                                62
                                                53
                                                                                                        (2)
# The following counts and displays how many elements of L5 has a determinated size.
# This can be used to guess what will be a good candidate for k.
count2 := [seq(0, i = 1 ..nops(L5[nops(L5)]))]:
for i from 1 to numelems(L5) do
count := nops(L5[i]) :
count2[count] := count2[count] + 1:
for i from 1 to nops(count2) do
printf ("There is %d configurations with %d valid polytopes.\n", count2[i], i);
od:
```

```
for J in L5 do
print(J);
od:
There is 0
                 configurations with 1 valid polytopes.
                 configurations with 2 valid polytopes.
There is 0
There is 6
                 configurations with 3 valid polytopes.
There is 0
                 configurations with 4 valid polytopes.
There is 23
                  configurations with 5 valid polytopes.
There is 0
                 configurations with 6 valid polytopes.
There is 20
                   configurations with 7 valid polytopes.
There is 0
                 configurations with 8 valid polytopes.
There is 4
                 configurations with 9 valid polytopes.
                           [[1, 2, 3, 12], [1, 2, 9, 12], [1, 2, 9, 12]]
                          [[1, 2, 3, 12], [1, 2, 10, 12], [1, 2, 10, 12]]
                          [[1, 2, 3, 12], [1, 2, 11, 12], [1, 2, 11, 12]]
                           [[1, 2, 3, 12], [1, 3, 8, 12], [1, 3, 8, 12]]
                           [[1, 2, 3, 12], [1, 3, 9, 12], [1, 3, 9, 12]]
                          [[1, 2, 3, 12], [1, 3, 10, 12], [1, 3, 10, 12]]
            [[1, 2, 3, 12], [1, 2, 9, 12], [1, 2, 9, 12], [1, 2, 11, 12], [1, 2, 11, 12]]
            [[1, 2, 3, 12], [1, 2, 9, 12], [1, 2, 10, 12], [1, 9, 10, 12], [2, 9, 10, 12]]
            [[1, 2, 3, 12], [1, 2, 9, 12], [1, 2, 11, 12], [1, 9, 11, 12], [2, 9, 11, 12]]
          [[1, 2, 3, 12], [1, 2, 10, 12], [1, 2, 11, 12], [1, 10, 11, 12], [2, 10, 11, 12]]
             [[1, 2, 3, 12], [1, 2, 11, 12], [1, 2, 11, 12], [1, 3, 8, 12], [1, 3, 8, 12]]
             [[1, 2, 3, 12], [1, 3, 8, 12], [1, 3, 8, 12], [1, 3, 10, 12], [1, 3, 10, 12]]
              [[1, 2, 3, 12], [1, 3, 8, 12], [1, 3, 9, 12], [1, 8, 9, 12], [3, 8, 9, 12]]
            [[1, 2, 3, 12], [1, 3, 8, 12], [1, 3, 10, 12], [1, 8, 10, 12], [3, 8, 10, 12]]
            [[1, 2, 3, 12], [1, 3, 9, 12], [1, 3, 10, 12], [1, 9, 10, 12], [3, 9, 10, 12]]
             [[1, 2, 8, 12], [1, 2, 10, 12], [1, 2, 10, 12], [1, 3, 8, 12], [2, 3, 8, 12]]
             [[1, 2, 8, 12], [1, 2, 11, 12], [1, 2, 11, 12], [1, 3, 8, 12], [2, 3, 8, 12]]
            [[1, 2, 9, 12], [1, 2, 11, 12], [1, 2, 11, 12], [1, 3, 9, 12], [2, 3, 9, 12]]
            [[1, 2, 10, 12], [1, 3, 8, 12], [1, 3, 8, 12], [1, 3, 10, 12], [2, 3, 10, 12]]
            [[1, 2, 10, 12], [1, 3, 8, 12], [1, 8, 10, 12], [2, 3, 8, 12], [2, 8, 10, 12]]
           [[1, 2, 10, 12], [1, 3, 8, 12], [1, 8, 10, 12], [2, 3, 10, 12], [3, 8, 10, 12]]
            [[1, 2, 10, 12], [1, 3, 9, 12], [1, 9, 10, 12], [2, 3, 9, 12], [2, 9, 10, 12]]
           [[1, 2, 10, 12], [1, 3, 9, 12], [1, 9, 10, 12], [2, 3, 10, 12], [3, 9, 10, 12]]
            [[1, 2, 11, 12], [1, 3, 8, 12], [1, 3, 8, 12], [1, 3, 11, 12], [2, 3, 11, 12]]
            [[1, 2, 11, 12], [1, 3, 8, 12], [1, 8, 11, 12], [2, 3, 8, 12], [2, 8, 11, 12]]
           [[1, 2, 11, 12], [1, 3, 8, 12], [1, 8, 11, 12], [2, 3, 11, 12], [3, 8, 11, 12]]
            [[1, 2, 11, 12], [1, 3, 9, 12], [1, 3, 9, 12], [1, 3, 11, 12], [2, 3, 11, 12]]
            [[1, 2, 11, 12], [1, 3, 9, 12], [1, 9, 11, 12], [2, 3, 9, 12], [2, 9, 11, 12]]
           [[1, 2, 11, 12], [1, 3, 9, 12], [1, 9, 11, 12], [2, 3, 11, 12], [3, 9, 11, 12]]
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- [[1, 2, 3, 12], [1, 2, 9, 12], [1, 2, 11, 12], [1, 9, 10, 12], [1, 10, 11, 12], [2, 9, 10, 12], [2, 10, 11, 12]]
- [[1, 2, 3, 12], [1, 3, 8, 12], [1, 3, 10, 12], [1, 8, 9, 12], [1, 9, 10, 12], [3, 8, 9, 12], [3, 9, 10, 12]]
- [[1, 2, 8, 12], [1, 2, 10, 12], [1, 2, 11, 12], [1, 3, 8, 12], [1, 10, 11, 12], [2, 3, 8, 12], [2, 10, 11, 12]]
- [[1, 2, 9, 12], [1, 2, 11, 12], [1, 2, 11, 12], [1, 3, 8, 12], [1, 8, 9, 12], [2, 3, 8, 12], [2, 8, 9, 12]]
- [[1, 2, 9, 12], [1, 2, 11, 12], [1, 2, 11, 12], [1, 3, 8, 12], [1, 8, 9, 12], [2, 3, 9, 12], [3, 8, 9, 12]]
- [[1, 2, 10, 12], [1, 3, 8, 12], [1, 8, 9, 12], [1, 9, 10, 12], [2, 3, 8, 12], [2, 8, 9, 12], [2, 9, 10, 12]]
- [[1, 2, 10, 12], [1, 3, 8, 12], [1, 8, 9, 12], [1, 9, 10, 12], [2, 3, 9, 12], [2, 9, 10, 12], [3, 8, 9, 12]]
- [[1, 2, 10, 12], [1, 3, 8, 12], [1, 8, 9, 12], [1, 9, 10, 12], [2, 3, 10, 12], [3, 8, 9, 12], [3, 9, 10, 12]]
- [[1, 2, 11, 12], [1, 3, 8, 12], [1, 3, 8, 12], [1, 3, 10, 12], [1, 10, 11, 12], [2, 3, 10, 12], [2, 10, 11, 12]]
- [[1, 2, 11, 12], [1, 3, 8, 12], [1, 3, 8, 12], [1, 3, 10, 12], [1, 10, 11, 12], [2, 3, 11, 12], [3, 10, 11, 12]]
- [[1, 2, 11, 12], [1, 3, 8, 12], [1, 3, 9, 12], [1, 3, 11, 12], [1, 8, 9, 12], [2, 3, 11, 12], [3, 8, 9, 12]]
- [[1, 2, 11, 12], [1, 3, 8, 12], [1, 8, 9, 12], [1, 9, 11, 12], [2, 3, 8, 12], [2, 8, 9, 12], [2, 9, 11, 12]]
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- [[1, 2, 11, 12], [1, 3, 8, 12], [1, 8, 10, 12], [1, 10, 11, 12], [2, 3, 8, 12], [2, 8, 10, 12], [2, 10, 11, 12]]
- [[1, 2, 11, 12], [1, 3, 8, 12], [1, 8, 10, 12], [1, 10, 11, 12], [2, 3, 10, 12], [2, 10, 11, 12], [3, 8, 10, 12]]
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[[1, 2, 11, 12], [1, 3, 8, 12], [1, 8, 9, 12], [1, 9, 10, 12], [1, 10, 11, 12], [2, 3, 8, 12], [2, 8, 9, 12], [2, 11, 12], [2, 11, 12], [2, 2, 3, 12], [2, 2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3, 12], [2, 3,
                        12], [2, 9, 10, 12], [2, 10, 11, 12]]
 [[1, 2, 11, 12], [1, 3, 8, 12], [1, 8, 9, 12], [1, 9, 10, 12], [1, 10, 11, 12], [2, 3, 9, 12], [2, 9, 10, 12], [1, 10, 11, 12], [2, 3, 9, 12], [2, 9, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], [2, 10, 12], 
                        12], [2, 10, 11, 12], [3, 8, 9, 12]]
 [[1, 2, 11, 12], [1, 3, 8, 12], [1, 8, 9, 12], [1, 9, 10, 12], [1, 10, 11, 12], [2, 3, 10, 12], [2, 10, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10
                        11, 12], [3, 8, 9, 12], [3, 9, 10, 12]]
 [[1, 2, 11, 12], [1, 3, 8, 12], [1, 8, 9, 12], [1, 9, 10, 12], [1, 10, 11, 12], [2, 3, 11, 12], [3, 8, 9, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 12], [1, 10, 11, 
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        (3)
                         12], [3, 9, 10, 12], [3, 10, 11, 12]]
# In the following we check for each element of L5 the conditions that are needed for it to be positively
                       decorated by Csimple.
all solutions := \{ \} :
   for J in L5 do
   # We only work with J in L5 with at least 2 \cdot \text{floor}\left(\frac{n}{2}\right) + 1 simplices.
   if numelems(J) \ge 2 \cdot floor(\frac{n}{2}) + 1 then
   Jused := [ ]:
# The variable "solutions" will have pairs [I,C].
# Each I is a list of (indexes of) simplices.
# The corresponding C is a list of expressions f1,..., fm such that the simplices
                       in I are simultaneously positively decorated by Csimple if and only if fl > 0..., fm > 0.
 # Each C has at least the conditions E, F and S (that is E > 0, F > 0, S
                             > 0) because these are total concentrations of chemical species.
# Each C also has 1-M[1],...,1-M[n-1] sinse these M[i] must be less than 1.
# We include in each C the expression 1 as well since the obvious condition 1 > 0 will help us to
                       eliminate bad candidates.
solutions := \{ [Jused, \{1, E, F, S, seq(1 - M[i], i = 0 ... n - 1) \}] \} :
solutionsaux := \{ \} :
                       # The next loop does the following. Start with the first element of J, if it gives viable solutions keep it
                       and discard it otherwise.
                      # Then if the second gives condities compatible with the first one keep it and discard it otherwise,
```

- and so on.

## for i in J do

# Now we compute two sets of conditions for j to be positively decorated by Csimple, conditionsnewa and conditionsnewb, these correspond to the two possibilites of the alternating signs of the four 3x3

```
for i from 1 to 4 do det[i] := Determinant(Csimple[1..3, subsop(i = NULL, j)]): od:
conditionsnewa := \{-det[1], det[2], -det[3], det[4]\};
conditionsnewb := \{det[1], -det[2], det[3], -det[4]\};
solutionsaux := \{ \} :
```

# Next we compare conditionsnewa and conditionsnewb with the previous conditions. We include

```
only one of them, if there is a compatible one.
for l in solutions do
 Jused := l[1]; conditions := l[2];
if evalb(numelems(conditions intersect conditions newa) \geq 1 and numelems(conditions
    intersect conditionsnewb ) \ge 1 ) = true then
solutionsaux := solutionsaux union \{ [Jused, conditions] \};
if evalb(numelems(conditions intersect conditionsnewb) = 0) = true then
solutions aux := solutions aux union \{ [[op(Jused), j], conditions union conditions newa] \};
if evalb(numelems(conditions intersect conditions newa) = 0) = true then
 solutions aux := solutions aux union \{ [[op(Jused), j], conditions union conditions newb] \};
fi:
od:
solutions := solutions aux;
 od:
 # Finally, in the variable "all solutions" we keep the candidates that give at least k=2 \cdot floor\left(\frac{n}{2}\right)
     +1 regions.
for k in solutions do
if numelems(k[1]) \ge 2 \cdot floor(\frac{n}{2}) + 1 then all solutions := all solutions union \{k\}; fi:
od:
 fi:
 od:
printf ("Number of solutions to try: %d.", numelems(allsolutions));
Number of solutions to try: 14.
# In this part we obtain L7 from "allsolutions".
# We do this searching in "allsolutions" for the elements for which there are viable parameters
    satisfying the conditions.
# This is the only numerical part of the whole script.
# In the end each J in L7 will contain:
\# J[1] = list of simplexes;
#J[2] = corresponding conditions;
\# J[3] = a list of real numbers which are viable values for the parameters.
interface(displayprecision = 6) : L7 := \{ \} :
for j in allsolutions do
conditions := j[2]:
Jused := j[1]:
# The next command "Minimize" is used to find a numerical solution for the condition.
# If the "Minimize" is able to find one solution then the conditions are viable and are included in L7.
# Since "Minimize" works only with closed conditions we use \geq \frac{1}{10000} instead of > 0.
# If "Minimize" is unable to find a solution it returns a error, because of that we need the "try"
```

```
command. In this case the conditions are discarded.
try
\mathit{Min} := \mathit{Minimize}\Big(1, \Big\{\mathit{seq}\Big(\mathit{conditions}[j] \geq \frac{1}{10000}, j = 1 \; .. \\ \mathit{numelems}(\mathit{conditions}) \;\Big)\Big\}, \mathit{assume}
     = nonnegative, iterationlimit = 100):
L7 := L7 \text{ union } \{ [j[1], j[2], Min[2]] \} :
catch:
end try:
end do:
    # The next loop for is used to remove the conditions 1 > 0, E > 0, ..., 1-M[i] > 0, M[i] > 0 from the
    elements of L7.
solutionsaux := \{ \} :
for k from 1 to numelems(L7) do
 solutions aux := solutions aux union \{[L7[k][1], L7[k][2] \text{ minus } \{1, E, F, S, seq(1-M[i], i=0 ..n \}\}
     -1), seq(M[i], i=0..n-1)}, L7[k][3]]}:
od:
 L7 := solutionsaux:
    # The next two loops are used to remove a set of conditions C if it is contained in another. In this
    way we get only maximal regions.
 solutionsaux := \{ \} :
for k from 1 to numelems(L7) do
aux := 0:
for j from k + 1 to numelems(L7) do
if evalb(L7[k][2]] subset L7[j][2]) then
aux := 1
fi:
od:
if aux = 0 then
solutions aux := solutions aux union \{ [L7[k][1], L7[k][2], L7[k][3]] \} :
fi:
od:
 L7 := solutionsaux:
printf [ "There are %d maximal regions, in which there are %d positive solutions each. \n",
    numelems(L7), 2 \cdot \text{floor}\left(\frac{n}{2}\right) + 1;
printf ("The original triangulations, simplices positively decorated, regions, and a point on each one
    are:");
```

for i from 1 to numelems (L7) do

# This line recovers the original triangulations from the final sets obtained.

```
Foundoriginaltriang (originals, Foundoriginaltriang (originals2, Foundoriginaltriang (originals3,
                      L7[i][1]));
L7[i][1];
L7[i][2];
L7[i][3];
od;
 There are 5 maximal regions, in which there are 5 positive
 solutions each.
The original triangulations, simplices positively decorated,
regions, and a point on each one are:
 [0, 1, 2, 7], [0, 1, 2, 11], [0, 1, 7, 8], [0, 1, 8, 11], [0, 6, 10, 11], [0, 8, 9, 11], [0, 9, 10, 11],
                       [1, 6, 10, 11], [1, 8, 9, 11], [1, 9, 10, 11]]
                                                                 [[1, 2, 3, 12], [1, 2, 9, 12], [1, 2, 11, 12], [1, 9, 10, 12], [1, 10, 11, 12]]
\{M_2 - M_1, M_2 - M_3, -EM_1 - FM_1 + E, EM_2 + FM_2 - E, -EM_3 - FM_3 + E, -SM_1 - F + S, -FM_2 - E, -FM_3 - FM_3 + E, -FM_4 - F + S, -FM_4 - F + S, -FM_4 - F + S, -FM_5 - F + S, -FM_
                        -SM_3 - F + S, EM_1 - EM_2 + FM_1 - FM_2 - SM_1 + SM_2, -EM_2 + EM_3 - FM_2 + FM_3
                        + S M_2 - S M_3
 [E=0.399860, F=0.000197, S=2.200280, M_0=0.999900, M_1=0.999258, M_2=0.999782, M_3=0.999782, M_3=0.999988, M_2=0.999988, M_3=0.999988, M_3=0.99998, M_3=0.9998, M_3=0.9988, M_3=0.9
                        =0.999258
 [[0, 2, 7, 11], [0, 6, 9, 11], [0, 7, 8, 11], [0, 8, 9, 11], [1, 2, 6, 9], [1, 2, 6, 11], [1, 6, 9, 10],
                       [2, 6, 9, 11], [2, 7, 8, 11], [2, 8, 9, 11]]
                                                                       [[1, 2, 3, 12], [1, 3, 8, 12], [1, 3, 10, 12], [1, 8, 9, 12], [1, 9, 10, 12]]
 \{M_0-M_1,M_2-M_1,S\,M_0-E,S\,M_2-E,E\,M_0+F\,M_0-E,-E\,M_1-F\,M_1+E,E\,M_2+F\,M_2+F\,M_2+F\,M_3+E\,M_2+F\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,M_3+E\,
                          -E, -EM_0 + EM_1 - FM_0 + FM_1 + SM_0 - SM_1, EM_1 - EM_2 + FM_1 - FM_2 - SM_1
                          +SM_2
 [E = 0.449981, F = 0.082246, S = 2.301131, M_0 = 0.917170, M_1 = 0.845280, M_2 = 0.910353, M_3 = 0.917170, M_1 = 0.845280, M_2 = 0.910353, M_3 = 0.917170, M_3 = 0.917170, M_4 = 0.845280, M_5 = 0.917170, M_8 = 0.917170, M
                         =0.999900
 [[0, 2, 7, 11], [0, 4, 8, 11], [0, 7, 8, 11], [1, 2, 8, 11], [1, 4, 8, 10], [1, 4, 8, 11], [1, 4, 10, 11],
                        [1, 6, 10, 11], [2, 7, 8, 11], [4, 6, 10, 11]]
                                                                       [[1, 2, 9, 12], [1, 2, 11, 12], [1, 2, 11, 12], [1, 3, 8, 12], [1, 8, 9, 12]]
 \{M_0 - M_1, SM_0 - E, EM_0 + FM_0 - E, -EM_1 - FM_1 + E, -EM_3 - FM_3 + E, -SM_1 - F + S, -EM_1 - F + S, -EM_2 - FM_3 + E, -SM_1 - F + S, -EM_2 - FM_3 + E, -SM_1 - F + S, -EM_2 - FM_3 + E, -SM_1 - F + S, -EM_2 - FM_3 + E, -SM_1 - F + S, -EM_2 - FM_3 + E, -SM_1 - F + S, -EM_2 - FM_3 + E, -SM_1 - F + S, -EM_2 - FM_3 + E, -SM_1 - F + S, -EM_2 - FM_3 + E, -SM_1 - F + S, -EM_2 - FM_3 + E, -SM_1 - F + S, -EM_2 - FM_3 + E, -SM_1 - F + S, -EM_2 - FM_3 + E, -SM_1 - F + S, -EM_2 - FM_3 + E, -SM_1 - F + S, -EM_2 - FM_3 + E, -SM_1 - F + S, -EM_2 - FM_3 + E, -SM_1 - F + S, -EM_2 - FM_3 + E, -SM_1 - F + S, -EM_2 - FM_3 + E, -SM_1 - FM_2 - FM_3 + E, -SM_2 - FM_3 - FM_3 + E, -SM_1 - FM_2 - FM_3 -
                       -S M_3 - F + S, -E M_0 + E M_1 - F M_0 + F M_1 + S M_0 - S M_1
 =0.999220
 [0, 2, 7, 11], [0, 4, 7, 11], [1, 2, 10, 11], [1, 6, 10, 11], [2, 4, 7, 9], [2, 4, 7, 11], [2, 4, 9, 11],
                       [2, 9, 10, 11], [4, 6, 10, 11], [4, 9, 10, 11]]
                                                                [[1, 2, 11, 12], [1, 3, 8, 12], [1, 3, 8, 12], [1, 3, 10, 12], [1, 10, 11, 12]]
 -F + S, -E M_2 + E M_3 - F M_2 + F M_3 + S M_2 - S M_3
```

```
 \begin{bmatrix} E = 0.399860, F = 0.000234, S = 2.200280, M_0 = 0.999900, M_1 = 0.999900, M_2 = 0.999708, M_3 \\ = 0.999166 \end{bmatrix}    \begin{bmatrix} [0, 2, 7, 11], [0, 6, 10, 11], [0, 7, 8, 11], [0, 8, 9, 11], [0, 9, 10, 11], [1, 2, 10, 11], [1, 6, 10, 11], [2, 7, 8, 11], [2, 8, 9, 11], [2, 9, 10, 11] \end{bmatrix}    \begin{bmatrix} [1, 2, 11, 12], [1, 3, 8, 12], [1, 8, 9, 12], [1, 9, 10, 12], [1, 10, 11, 12] \end{bmatrix}   \{ M_0 - M_1, M_2 - M_1, M_2 - M_3, S M_0 - E, E M_0 + F M_0 - E, -E M_1 - F M_1 + E, E M_2 + F M_2 - E, -E M_3 - F M_3 + E, -S M_3 - F + S, -E M_0 + E M_1 - F M_0 + F M_1 + S M_0 - S M_1, E M_1 - E M_2 + F M_1 - F M_2 - S M_1 + S M_2, -E M_2 + E M_3 - F M_2 + F M_3 + S M_2 - S M_3 \}   \begin{bmatrix} E = 0.399861, F = 0.000213, S = 2.200280, M_0 = 0.999746, M_1 = 0.999217, M_2 = 0.999746, M_3 \\ = 0.999217 \end{bmatrix}
```