```
eclipse sort.dat
 9 11, 12 16:46
                                                                  Page 1/145
< Calculation of the overlap vector >
* 0 <oovv/oovv>
    1.00000000) T2(o1,o2,a,c) E2(i,k,o1,o2)
    1.00000000) T2(o1,o2,c,a) E2(i,k,o2,o1)
Decompose RDMs .....
< RESULT2 >
   Setting up parameters as default ....
! * 0 terms are replaced in the linking process ....
! 02(i,k,a,c) <--
! ( 1.00000000) D2(i,o2,k,o1) T2(o2,o1,a,c)
! Indices of BareAmp are rotated to match with LHS.
Case 0 ..... O2(i,k,a,c) <---- ( 1.00000000) D2(i,o2,k,o1) T2(o2,o1,a,c)
! Polynomial order is O(o^4v^2)
! Maximum memory usage is O(o^2v^1)
! The optimal choice is .....
1: O2(i,k,a,c) < -- (1.00000000) D2(i,o2,k,o1) T2(o2,o1,a,c)
! Scaling
             : O(o^4v^2)
! Max size of X : o^2v^1
! * Begin scaling analysis .... *
for c in {vir}:
  Read T2 from GA for c
 Read 02 from GA for c
 Declare 02 as a o^2v^1 tensor
 O2_{(c)}(i, k, a) += sum(o2,o1) D2(i,o2,k,o1) * T2(o2,o1,a,)
 Accumulate O2_(c)(i,k,a) for c
! 02(i,k,a,c) <--
! (1.00000000) D2(i,o1,k,o2) T2(o2,o1,c,a)
Case 0 ..... O2(i,k,c,a) < ---- ( 1.00000000) D2(i,o1,k,o2) T2(o2,o1,c,a)
! Polynomial order is O(o^4v^2)
! Maximum memory usage is O(o^2)
! The optimal choice is .....
1: O2(i,k,c,a) < -- (1.00000000) D2(i,o1,k,o2) T2(o2,o1,c,a)
! Scaling
            : O(o^4v^2)
! Max size of X : o^2
! * Begin scaling analysis .... *
for c in {vir}:
 Read 02 from GA for c
 for a in {vir}:
   Read T2 from GA for a
    Declare O2 as a o^2 tensor
   O2_{(c)}(i, k, a) += sum(o1,o2) D2(i,o1,k,o2) * T2(o2,o1,c,)
```

```
eclipse sort.dat
 9 11, 12 16:46
                                                                   Page 2/145
  Accumulate 02 (c)(i,k,a) for c
* 1 <000v/000v>
  1.00000000) T2(o1,o2,o3,a) E3(i,k,o3,m,o2,o1)
   1.00000000) T2(o1,o2,m,a) E2(i,k,o1,o2)
Decompose RDMs .....
< RESULT2 >
   0: (1.00000000) D3(i,m,k,o2,o1,o3) T2(o3,o2,o1,a)
   1: (1.00000000) D2(i,o1,k,o2) T2(o1,o2,m,a)
Setting up parameters as default ....
! * 0 terms are replaced in the linking process ....
! No.0
! O2(i,k,m,a) <--
! ( 1.00000000) D3(i,m,k,o2,o1,o3) T2(o3,o2,o1,a)
! Indices of BareAmp are rotated to match with LHS.
Case 0 ..... O2(i,m,k,a) < ---- (1.00000000) D3(i,m,k,o2,o1,o3) T2(o3,o2,o3)
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^3)
! The optimal choice is .....
1: O2(i,m,k,a) <-- ( 1.00000000) D3(i,m,k,o2,o1,o3) T2(o3,o2,o1,a)
             : O(o^6v^1)
! Max size of X : o^3
! * Begin scaling analysis .... *
for a in {vir}:
 Read T2 from GA for a
  Read O2 from GA for a
  Declare 02 as a o^3 tensor
 O2_{(a)}(i, k, m) += sum(o2,o1,o3) D3(i,m,k,o2,o1,o3) * T2(o3,o2,o1,)
 Accumulate O2_(a)(i,k,m) for a
! No.1
! O2(i,k,m,a) <--
! ( 1.00000000) D2(i,o1,k,o2) T2(o1,o2,m,a)
! Indices of BareAmp are rotated to match with LHS.
Case 0 ..... O2(i,k,m,a) < ---- ( 1.00000000) D2(i,o1,k,o2) T2(o1,o2,m,a)
! Polynomial order is O(o^5v^1)
! Maximum memory usage is O(o^3)
! The optimal choice is .....
1: O2(i,k,m,a) < -- (1.00000000) D2(i,o1,k,o2) T2(o1,o2,m,a)
! Scaling
              : O(o^5v^1)
! Max size of X : o^3
! * Begin scaling analysis .... *
for a in {vir}:
```

```
eclipse_sort.dat
 9 11, 12 16:46
                                                                     Page 3/145
 Read T2 from GA for a
 Read O2 from GA for a
 Declare 02 as a o^3 tensor
 O2(a)(i, k, m) += sum(o1,o2) D2(i,o1,k,o2) * T2(o1,o2,m,)
 Accumulate O2_(a)(i,k,m) for a
< Calculation of the diagonal elements starts >
* 1 L:oovv/R:oovv
     0.50000000) V2(c1,c2,c3,c4) E4(c1,c2,i,k,c3,c4,i,k)
    0.50000000) V2(c1,c2,c3,c4) kDelta(a,c) kDelta(a,c) E4(c1,c2,i,k,c3,c4,k,i)
     0.50000000) V2(c1,o1,c2,o2) E4(c1,i,k,o1,c2,i,k,o2)
    0.50000000) V2(c1,o1,c2,o2) kDelta(a,c) kDelta(a,c) E4(c1,i,k,o1,c2,k,i,o2)
     0.50000000) V2(c1,c2,o2,o1) E4(c1,i,k,o1,o2,i,k,c2)
    0.50000000) V2(c1,c2,o2,o1) kDelta(a,c) kDelta(a,c) E4(c1,i,k,o1,o2,k,i,c2)
     0.50000000) V2(c1,a,c2,c) kDelta(a,c) E3(c1,i,k,c2,k,i)
    0.50000000) V2(c1,a,c2,a) E3(c1,i,k,c2,i,k)
    0.50000000) V2(c1,c,c2,c) E3(c1,i,k,c2,i,k)
    0.50000000) V2(c1,a,c2,c) kDelta(a,c) E3(c1,i,k,c2,k,i)
    0.50000000) V2(c1,c2,a,c) kDelta(a,c) E3(c1,i,k,i,k,c2)
     0.50000000) V2(c1,c2,a,a) E3(c1,i,k,i,c2,k)
    0.50000000) V2(c1,c2,c,c) E3(c1,i,k,k,i,c2)
     0.50000000) V2(c1,c2,c,a) kDelta(a,c) E3(c1,i,k,k,c2,i)
     0.50000000) V2(c1,c2,o2,o1) E4(c1,i,k,o1,o2,i,k,c2)
     0.50000000) V2(c1,c2,o2,o1) kDelta(a,c) kDelta(a,c) E4(c1,i,k,o1,o2,k,i,c2)
     0.50000000) V2(c1,o1,c2,o2) E4(c1,i,k,o1,c2,i,k,o2)
    0.50000000) V2(c1,o1,c2,o2) kDelta(a,c) kDelta(a,c) E4(c1,i,k,o1,c2,k,i,o2)
     0.50000000) V2(o1,o2,o3,o4) E4(i,k,o1,o2,i,k,o3,o4)
    0.50000000) V2(o1,o2,o3,o4) kDelta(a,c) kDelta(a,c) E4(i,k,o1,o2,k,i,o3,o4)
      0.50000000) \ \ V2(o1,a,o2,c) \ \ kDelta(a,c) \ \ E3(i,k,o1,k,i,o2) 
    0.50000000) V2(o1,a,o2,a) E3(i,k,o1,i,k,o2)
    0.50000000) V2(o1,c,o2,c) E3(i,k,o1,i,k,o2)
     0.50000000) V2(o1,a,o2,c) kDelta(a,c) E3(i,k,o1,k,i,o2)
     0.50000000) V2(o1,o2,a,c) kDelta(a,c) E3(i,k,o1,k,o2,i)
     0.50000000) V2(o1,o2,a,a) E3(i,k,o1,o2,k,i)
     0.50000000) V2(o1,o2,c,c) E3(i,k,o1,i,o2,k)
    0.50000000) V2(o1,o2,c,a) kDelta(a,c) E3(i,k,o1,o2,i,k)
    0.50000000) V2(c1,c2,a,c) kDelta(a,c) E3(c1,i,k,i,k,c2)
     0.50000000) V2(c1,c2,a,a) E3(c1,i,k,i,c2,k)
    0.50000000) V2(c1,c2,c,c) E3(c1,i,k,k,i,c2)
    0.50000000) V2(c1,c2,c,a) kDelta(a,c) E3(c1,i,k,k,c2,i)
     0.50000000) V2(c1,a,c2,c) kDelta(a,c) E3(c1,i,k,c2,k,i)
    0.50000000) V2(c1,a,c2,a) E3(c1,i,k,c2,i,k)
    0.50000000) V2(c1,c,c2,c) E3(c1,i,k,c2,i,k)
     0.50000000) V2(c1,a,c2,c) kDelta(a,c) E3(c1,i,k,c2,k,i)
     0.50000000) V2(o1,o2,a,c) kDelta(a,c) E3(i,k,o1,k,o2,i)
     0.50000000) V2(o1,o2,a,a) E3(i,k,o1,o2,k,i)
     0.50000000) V2(o1,o2,c,c) E3(i,k,o1,i,o2,k)
    0.50000000) V2(o1,o2,c,a) kDelta(a,c) E3(i,k,o1,o2,i,k)
    0.50000000) V2(o1,a,o2,c) kDelta(a,c) E3(i,k,o1,k,i,o2)
    0.50000000) V2(o1,a,o2,a) E3(i,k,o1,i,k,o2)
     0.50000000) V2(o1,c,o2,c) E3(i,k,o1,i,k,o2)
     0.50000000) V2(o1,a,o2,c) kDelta(a,c) E3(i,k,o1,k,i,o2)
     0.50000000) V2(a,c,a,c) E2(i,k,i,k)
    0.50000000) V2(a,a,c,c) E2(i,k,k,i)
    0.50000000) V2(a,a,c,c) E2(i,k,k,i)
     0.50000000) V2(a,c,a,c) E2(i,k,i,k)
Decompose RDMs ....
```

9 11, 12 1	6:46	eclipse_sort.dat	Page 4/145
			-
<pre>< RESULT > 0 : (1 : (2 : (3 : (4 : (5 : (6 : (7 : (8 : (9 : (10 : (11 : (12 : () }</pre>	2.00000000) 1.00000000) 2.00000000) 1.00000000) 1.00000000) 2.00000000) -1.00000000) -1.00000000) 2.000000000)	D2(i,k,i,k) h(c1,c1) D2(i,k,k,i) h(c1,c1) kDelta(a,c) kDelta D3(i,k,o1,i,k,o2) h(o1,o2) D3(i,k,o1,k,i,o2) h(o1,o2) kDelta(a,c) B D2(i,k,i,k) h(a,c) kDelta(a,c) D2(i,k,i,k) h(a,a) D2(i,k,i,k) h(c,c) D2(i,k,i,k) V2(c2,c1,c2,c1) D2(i,k,i,k) V2(c2,c2,c1,c1) D2(i,k,i,k) V2(c2,c2,c1,c2) D2(i,k,k,i) V2(c2,c1,c2,c1) kDelta(a,c) D2(i,k,k,i) V2(c1,c1,c2,c2) kDelta(a,c) D3(i,k,o2,i,k,o1) V2(c1,o2,c1,o1) D3(i,k,o1,k,i,o2) V2(c1,o1,c1,o2) kDelta	kDelta(a,c) kDelta(a,c) kDelta(a,c)
13 : (14 : (D3(i,k,o2,i,k,o1) V2(c1,c1,o2,o1) D3(i,k,o1,k,i,o2) V2(c1,c1,o1,o2) kDelta	a(a,c) kDelta(a,
15 : (16 : (17 : (18 : (19 : (20 : (21 : (22 : (2.00000000) 2.00000000) -2.00000000) -1.00000000) 0.50000000)	D2(i,k,k,i) V2(cl,a,cl,c) kDelta(a,c) D2(i,k,i,k) V2(cl,a,cl,a) D2(i,k,i,k) V2(cl,c,cl,c) D2(i,k,i,k) V2(cl,cl,a,c) kDelta(a,c) D2(i,k,i,k) V2(cl,cl,a,a) D2(i,k,i,k) V2(cl,cl,a,a) D2(i,k,i,k) V2(cl,cl,c,c) D4(i,k,ol,o2,i,k,o3,o4) V2(ol,o2,o3,o4) D4(i,k,ol,o2,k,i,o3,o4) V2(ol,o2,o3,o4)	kDelta(a,c) kDe
lta(a,c) 23 : (24 : (25 : (26 : (27 : (28 : (29 : (30 : (1.00000000) 1.00000000) 2.00000000) 1.00000000) 1.00000000)	D3(i,k,o1,k,i,o2) V2(o1,a,o2,c) kDelta(a) D3(i,k,o2,i,k,o1) V2(o2,a,o1,a) D3(i,k,o1,i,k,o2) V2(o1,c,o2,c) D3(i,k,o2,k,o1,i) V2(o2,o1,a,c) kDelta(a) D3(i,k,o2,o1,k,i) V2(o2,o1,a,a) D3(i,k,o1,i,o2,k) V2(o1,o2,c,c) D2(i,k,i,k) V2(a,c,a,c) D2(i,k,k,i) V2(a,a,c,c)	
<pre>< RESULT2 0 : (1 : (2 : (3 : (4 : (5 : (6 : (7 : (8 : (9 : (10 : (11 : (12 : (2 : (3 : (4 : (5 : (7 : (8 : (9 : (10 : (11 : (12 : (</pre>	2.00000000) 2.00000000) 1.00000000) 1.00000000) 1.00000000) 1.00000000) 2.00000000) -1.00000000) -1.00000000) -1.00000000) 2.000000000)	D2(i,i,k,k) h(c1,c1) D2(i,k,k,i) h(c1,c1) kDelta(a,c) kDelta D3(i,i,k,k,o1,o2) h(o1,o2) D3(i,k,k,i,o1,o2) h(o1,o2) kDelta(a,c) l D2(i,k,k,i) h(a,c) kDelta(a,c) D2(i,i,k,k) h(a,a) D2(i,i,k,k) h(c,c) D2(i,i,k,k) V2(c1,c1,c2,c2) D2(i,i,k,k) V2(c1,c2,c1,c2) D2(i,k,k,i) V2(c1,c1,c2,c2) kDelta(a,c) D2(i,k,k,i) V2(c1,c2,c1,c2) kDelta(a,c) D2(i,k,k,i) V2(c1,c2,c1,c2) kDelta(a,c) D3(i,i,k,k,o1,o2) V2(c1,c1,o1,o2) kDelta(a,c) D3(i,k,k,i,o1,o2) V2(c1,c1,o1,o2) kDelta(a,c)	kDelta(a,c) kDelta(a,c) kDelta(a,c)
13 : (14 : (D3(i,i,k,k,o1,o2) V2(c1,o1,c1,o2) D3(i,k,k,i,o1,o2) V2(c1,o1,c1,o2) kDelta	a(a,c) kDelta(a,
15 : (16 : (17 : (18 : (19 : (20 : (21 : (22 : (lta(a,c)	2.00000000) 2.00000000) -2.00000000) -1.00000000) 0.50000000)	D2(i,k,k,i) V2(cl,cl,a,c) kDelta(a,c) D2(i,i,k,k) V2(cl,cl,a,a) D2(i,i,k,k) V2(cl,cl,c,c) D2(i,k,k,i) V2(cl,a,cl,c) kDelta(a,c) D2(i,i,k,k) V2(cl,a,cl,a) D2(i,i,k,k) V2(cl,a,cl,a) D2(i,i,k,k) V2(cl,a,cl,c) D4(i,i,k,k) V2(cl,c,cl,c) D4(i,i,k,k,cl,o3,o2,o4) V2(ol,o3,o2,o4) D4(i,k,k,i,o1,o3,o2,o4) V2(ol,o3,o2,o4)	kDelta(a,c) kDe
23 : (24 : (25 : (1.00000000)	D3(i,k,k,i,o1,o2) V2(o1,o2,a,c) kDelta(a D3(i,i,k,k,o1,o2) V2(o1,o2,a,a) D3(i,i,k,k,o1,o2) V2(o1,o2,c,c)	a,c)

```
eclipse_sort.dat
 9 11, 12 16:46
                                                                          Page 5/145
              2.00000000) D3(i,k,k,o1,o2,i) V2(o1,c,o2,a) kDelta(a,c)
   26 : (
             1.00000000) D3(i,o1,k,k,o2,i) V2(o1,a,o2,a)
   2.7 : (
   28 : (
             1.00000000) D3(i,i,k,o1,o2,k) V2(o1,c,o2,c)
   29 : (
             1.00000000) D2(i,i,k,k) V2(a,a,c,c)
   30 : (
             1.00000000) D2(i,k,k,i) V2(a,c,a,c)
< RESULT >
    0: (
             2.00000000) D2(i,i,k,k) h(c1,c1)
    1: (
              2.00000000) D2(i,k,k,i) h(c1,c1) kDelta(a,c) kDelta(a,c)
             1.00000000) D3(i,i,k,k,o1,o2) h(o1,o2) 
1.00000000) D3(i,k,k,i,o1,o2) h(o1,o2) kDelta(a,c) kDelta(a,c)
    2: (
    3: (
    4: (
             2.00000000) D2(i,k,k,i) h(a,c) kDelta(a,c)
             1.00000000) D2(i,i,k,k) h(a,a)
1.00000000) D2(i,i,k,k) h(c,c)
    5 : (
    6 : (
            2.00000000) D2(i,i,k,k) V2(c1,c1,c2,c2)
-1.00000000) D2(i,i,k,k) V2(c1,c2,c1,c2)
    7:(
    8 : (
           2.00000000) D2(i,k,k,i) V2(c1,c1,c2,c2) kDelta(a,c) kDelta(a,c)
    9: (
   10: (
            -1.00000000) D2(i,k,k,i) V2(c1,c2,c1,c2) kDelta(a,c) kDelta(a,c)
   11: ( 2.00000000) D3(i,i,k,k,o1,o2) V2(c1,c1,o1,o2)
12: ( 2.00000000) D3(i,k,k,i,o1,o2) V2(c1,c1,o1,o2) kDelta(a,c) kDelta(a,
c)
   13 : (-1.00000000) D3(i,i,k,k,o1,o2) V2(c1,o1,c1,o2)
            -1.00000000) D3(i,k,k,i,o1,o2) V2(c1,o1,c1,o2) kDelta(a,c) kDelta(a,
   14: (
c)
             4.00000000) D2(i,k,k,i) V2(c1,c1,a,c) kDelta(a,c)
   16 : ( 2.00000000) D2(i,i,k,k) V2(c1,c1,a,a)
   17 : (
            2.00000000) D2(i,i,k,k) V2(c1,c1,c,c)
   18 : (
            -2.00000000) D2(i,k,k,i) V2(c1,a,c1,c) kDelta(a,c)
            -1.00000000) D2(i,i,k,k) V2(c1,a,c1,a)
   19 : (
   20 : (
            -1.00000000) D2(i,i,k,k) V2(c1,c,c1,c)
   21 : (
            0.50000000) D4(i,i,k,k,o1,o3,o2,o4) V2(o1,o3,o2,o4) 
0.50000000) D4(i,k,k,i,o1,o3,o2,o4) V2(o1,o3,o2,o4) kDelta(a,c) kDe
   22: (
lta(a,c)
   23 : (
             2.00000000) D3(i,k,k,i,o1,o2) V2(o1,o2,a,c) kDelta(a,c)
             1.00000000) D3(i,i,k,k,o1,o2) V2(o1,o2,a,a)
   24: (
             1.00000000) D3(i,i,k,k,o1,o2) V2(o1,o2,c,c)
   25 : (
             2.00000000) D3(i,k,k,o1,o2,i) V2(o1,c,o2,a) kDelta(a,c)
1.00000000) D3(i,o1,k,k,o2,i) V2(o1,a,o2,a)
1.00000000) D3(i,i,k,o1,o2,k) V2(o1,c,o2,c)
1.00000000) D2(i,i,k,k) V2(a,a,c,c)
   27 : (
  28: ( 1.00000000) D3(i,i,k,o1,o2,k) V2(o1
29: ( 1.00000000) D2(i,i,k,k) V2(a,a,c,c)
30: ( 1.00000000) D2(i,k,k,i) V2(a,c,a,c)
Setting up parameters as default ....
       +:+
    :#::+::# +#++:++# +#+ +:+ +#+ +#+ +#+ +:+
  +#+ +#+ +#+ +#+ +#+ +#+
                                    #+# #+#
  #+#
             #+#
                         #+#
                                                  #+#
                                                          #+#
 ###
             ### ###
! * 16 terms are replaced in the linking process ....
The linked formulas ....
0 : ( 2.00000000) Y0 D2(i,i,k,k)
         2.00000000) Y1 D2(i,k,k,i) kDelta(a,c) kDelta(a,c)
1: (
        1.00000000) D3(i,i,k,k,o1,o2) h(o1,o2)
2: (
        1.00000000) D3(i,k,k,i,o1,o2) h(o1,o2) kDelta(a,c) kDelta(a,c)
3 : (
4 : ( 2.00000000) D2(i,k,k,i) h(a,c) kDelta(a,c) 
5 : ( 1.00000000) D2(i,i,k,k) h(a,a)
        1.00000000) D2(i,i,k,k) h(c,c)
6: (
         2.00000000) Y2 D2(i,i,k,k)
7: (
        -1.00000000) Y3 D2(i,i,k,k)
         2.00000000) Y4 D2(i,k,k,i) kDelta(a,c) kDelta(a,c)
9: (
10 : ( -1.00000000) Y5 D2(i,k,k,i) kDelta(a,c) kDelta(a,c)
11: (
        2.00000000) D3(i,i,k,k,o1,o2) Y6(o1,o2)
          2.00000000) D3(i,k,k,i,o1,o2) Y7(o1,o2) kDelta(a,c) kDelta(a,c)
12: (
```

```
eclipse sort.dat
  9 11, 12 16:46
                                                                            Page 6/145
13: (
          -1.00000000) D3(i,i,k,k,o1,o2) Y8(o1,o2)
          -1.00000000) D3(i,k,k,i,o1,o2) Y9(o1,o2) kDelta(a,c) kDelta(a,c)
14 : (
          4.00000000) D2(i,k,k,i) Y10(a,c) kDelta(a,c) 2.00000000) D2(i,i,k,k) Y11(a,a)
15 : (
16: (
         2.00000000) D2(i,i,k,k) Y12(c,c)
17 : (
18 : (
         -2.00000000) D2(i,k,k,i) Y13(a,c) kDelta(a,c) -1.00000000) D2(i,i,k,k) Y14(a,a)
19: (
20 : (
          -1.00000000) D2(i,i,k,k) Y15(c,c)
21 : (
          0.50000000) D4(i,i,k,k,o1,o3,o2,o4) V2(o1,o3,o2,o4)
22 : (
           0.50000000) D4(i,k,k,i,o1,o3,o2,o4) V2(o1,o3,o2,o4) kDelta(a,c) kDelta
(a,c)
23 : (
          2.00000000) D3(i,k,k,i,o1,o2) V2(o1,o2,a,c) kDelta(a,c)
24 : (
          1.00000000) D3(i,i,k,k,o1,o2) V2(o1,o2,a,a)
          1.00000000) D3(i,i,k,k,o1,o2) V2(o1,o2,c,c)
25 : (
           2.00000000) D3(i,k,k,o1,o2,i) V2(o1,c,o2,a) kDelta(a,c) 1.00000000) D3(i,o1,k,k,o2,i) V2(o1,a,o2,a) 1.00000000) D3(i,i,k,o1,o2,k) V2(o1,c,o2,c)
26 : (
2.7 : (
28 : (
29 : ( 1.00000000) D2(i,i,k,k) V2(a,a,c,c)
30 : (1.00000000) D2(i,k,k,i) V2(a,c,a,c)
The content of each effective tensor ....
Y0 <-- ( 1.00000000) h(c1,c1)
Y1 <-- ( 1.00000000) h(c1,c1)
Y2 <-- (
            1.00000000) V2(c1,c1,c2,c2)
Y3 <-- ( 1.00000000) V2(c1,c2,c1,c2)
Y4 <-- (
            1.00000000) V2(c1,c1,c2,c2)
            1.00000000) V2(c1,c2,c1,c2)
1.00000000) V2(c1,c1,c1,c2)
1.00000000) V2(c1,c1,c1,c2)
Y5 <-- (
Y6 <-- (
Y7 <-- (
Y8 <-- (
            1.00000000) V2(c1,o1,c1,o2)
Y9 <-- (
            1.00000000) V2(c1,o1,c1,o2)
Y10 <-- ( 1.00000000) V2(c1,c1,a,c)
              1.00000000) V2(c1,c1,a,a)
1.00000000) V2(c1,c1,c,c)
Y11 <-- (
Y12 <-- (
              1.00000000) V2(c1,a,c1,c)
Y13 <-- (
              1.00000000) V2(c1,a,c1,a)
Y14 <-- (
Y15 <-- (
              1.00000000) V2(c1,c,c1,c)
! No.0
! Hdiag(i,k,a,c) <--
! ( 2.00000000) Y0 D2(i,i,k,k)
! * Begin scaling analysis .... *
Declare YO as a scalar
for c in {vir}:
 Read Hdiag from GA for c
  Hdiag_{(c)}(i, k, a) += 2 Y0 sum() D2(i,i,k,k)
  Accumulate Hdiag (c)(i,k,a) for c
! Hdiag(i,k,a,c) <--
! ( 2.00000000) Y1 D2(i,k,k,i) kDelta(a,c) kDelta(a,c)
! Kronecker's delta removed.
! * Begin scaling analysis .... *
Declare Y1 as a scalar
for a in {vir}:
 Read Hdiag from GA for a
  Hdiag_{(a)}(i, k, a) += 2 Y1 sum() D2(i,k,k,i)
  Accumulate Hdiag_(a)(i,k,a) for a
```

	9 11, 12 16:46 eclipse_sort.dat	Page 7/145
!	No.2 Hdiag(i,k,a,c) < (1.00000000) D3(i,i,k,k,o1,o2) h(o1,o2) * Begin scaling analysis *	
f	or c in {vir}: Read Hdiag from GA for c Hdiag_(c)(i, k, a) += sum(o1,o2) D3(i,i,k,k,o1,o2) * h(o1,o2) Accumulate Hdiag_(c)(i,k,a) for c	
!!!	No.3 Hdiag(i,k,a,c) < (1.00000000) D3(i,k,k,i,o1,o2) h(o1,o2) kDelta(a,c) kDelta(a,c Kronecker's delta removed. * Begin scaling analysis *)
f	or a in {vir}: Read Hdiag from GA for a Hdiag_(a)(i, k, a) += sum(o1,o2) D3(i,k,k,i,o1,o2) * h(o1,o2) Accumulate Hdiag_(a)(i,k,a) for a	
!!	No.4 Hdiag(i,k,a,c) < (2.00000000) D2(i,k,k,i) h(a,c) kDelta(a,c) Kronecker's delta removed. * Begin scaling analysis *	
	or a in {vir}: Read Hdiag from GA for a Hdiag_(a)(i, k, a) += 2 sum() D2(i,k,k,i) * h(a,a) Accumulate Hdiag_(a)(i,k,a) for a	
!!	No.5 Hdiag(i,k,a,c) < (1.00000000) D2(i,i,k,k) h(a,a) * Begin scaling analysis *	
f	or c in {vir}: Read Hdiag from GA for c Hdiag_(c)(i, k, a) += sum() D2(i,i,k,k) * h(a,a) Accumulate Hdiag_(c)(i,k,a) for c	
!		
!	No.6 Hdiag(i,k,a,c) < (1.00000000) D2(i,i,k,k) h(c,c) * Begin scaling analysis *	
f	or c in {vir}: Read Hdiag from GA for c Hdiag_(c)(i, k, a) += sum() D2(i,i,k,k) * h(c,c) Accumulate Hdiag_(c)(i,k,a) for c	
!		
!	No.7	

9 11, 12 16:46	eclipse_sort.dat	Page 8/145
! Hdiag(i,k,a,c) < ! (2.00000000) Y2 D2(! * Begin scaling analysi		
Declare Y2 as a scalar for c1 in {core}: Read V2 from GA for c1		
<pre>for c in {vir}: Read Hdiag from GA for Hdiag_(c)(i, k, a) += 2 Accumulate Hdiag_(c)(i,</pre>	2 Y2 sum() D2(i,i,k,k)	
!		
! No.8 ! Hdiag(i,k,a,c) < ! (-1.00000000) Y3 D2(! * Begin scaling analysi		
Declare Y3 as a scalar for c1 in {core}: Read V2 from GA for c1		
<pre>for c in {vir}: Read Hdiag from GA for Hdiag_(c)(i, k, a) += N Accumulate Hdiag_(c)(i,</pre>	Y3 sum() D2(i,i,k,k)	
!		
! No.9 ! Hdiag(i,k,a,c) < ! (2.00000000) Y4 D2(! Kronecker's delta remov ! * Begin scaling analysi		
Declare Y4 as a scalar for c1 in {core}: Read V2 from GA for c1		
for a in {vir}: Read Hdiag from GA for Hdiag_(a)(i, k, a) += 2 Accumulate Hdiag_(a)(i,	2 Y4 sum() D2(i,k,k,i)	
!		
! No.10 ! Hdiag(i,k,a,c) < ! (-1.00000000) Y5 D2(! Kronecker's delta remov ! * Begin scaling analysi		
Declare Y5 as a scalar for c1 in {core}: Read V2 from GA for c1		
for a in {vir}: Read Hdiag from GA for Hdiag_(a)(i, k, a) += N Accumulate Hdiag_(a)(i,	Y5 sum() D2(i,k,k,i)	
!		

```
eclipse sort.dat
 9 11, 12 16:46
                                                                    Page 9/145
! No.11
! Hdiag(i,k,a,c) <--
! ( 2.00000000) D3(i,i,k,k,o1,o2) Y6(o1,o2)
! * Begin scaling analysis .... *
Declare Y6 as a tensor
for c1 in {core}:
 Read V2 from GA for c1
for c in {vir}:
 Read Hdiag from GA for c
 Hdiag_{(c)}(i, k, a) += 2 sum(o1,o2) D3(i,i,k,k,o1,o2) * Y6(o1,o2)
 Accumulate Hdiag (c)(i,k,a) for c
! No.12
! Hdiag(i,k,a,c) <--
! ( 2.00000000) D3(i,k,k,i,o1,o2) Y7(o1,o2) kDelta(a,c) kDelta(a,c)
! Kronecker's delta removed.
! * Begin scaling analysis .... *
Declare Y7 as a tensor
for c1 in {core}:
 Read V2 from GA for c1
for a in {vir}:
 Read Hdiag from GA for a
 Hdiag_(a)(i, k, a) += 2 sum(o1,o2) D3(i,k,k,i,o1,o2) * Y7(o1,o2)
 Accumulate Hdiag (a)(i,k,a) for a
! No.13
! Hdiag(i,k,a,c) <--
! ( -1.00000000) D3(i,i,k,k,o1,o2) Y8(o1,o2)
! * Begin scaling analysis .... *
Declare Y8 as a tensor
for c1 in {core}:
 Read V2 from GA for c1
for c in {vir}:
 Read Hdiag from GA for c
 Hdiag_{(0)}(i, k, a) += sum(01,02) D3(i,i,k,k,01,02) * Y8(01,02)
 Accumulate Hdiag_(c)(i,k,a) for c
! No.14
! Hdiag(i,k,a,c) <--
! ( -1.00000000) D3(i,k,k,i,o1,o2) Y9(o1,o2) kDelta(a,c) kDelta(a,c)
! Kronecker's delta removed.
! * Begin scaling analysis .... *
Declare Y9 as a tensor
for c1 in {core}:
 Read V2 from GA for c1
for a in {vir}:
 Read Hdiag from GA for a
 Hdiag_{(a)}(i, k, a) += sum(01,02) D3(i,k,k,i,01,02) * Y9(01,02)
 Accumulate Hdiag_(a)(i,k,a) for a
```

```
eclipse sort.dat
  9 11, 12 16:46
                                                                    Page 10/145
! No.15
! Hdiaq(i,k,a,c) <--
! ( 4.00000000) D2(i,k,k,i) Y10(a,c) kDelta(a,c)
! Kronecker's delta removed.
! * Begin scaling analysis .... *
Declare Y10 as a tensor
for c1 in {core}:
   Read V2 from GA for c1
for a in {vir}:
  Read Hdiag from GA for a
  Hdiag_(a)(i, k, a) += 4 sum() D2(i,k,k,i) * Y10(a,a)
  Accumulate Hdiag_(a)(i,k,a) for a
! No.16
! Hdiaq(i,k,a,c) <--
! ( 2.00000000) D2(i,i,k,k) Y11(a,a)
! * Begin scaling analysis .... *
Declare Y11 as a tensor
for c1 in {core}:
 Read V2 from GA for c1
for c in {vir}:
 Read Hdiag from GA for c
  Hdiag_(c)(i, k, a) += 2 sum() D2(i,i,k,k) * Y11(a,a)
  Accumulate Hdiag_(c)(i,k,a) for c
! No.17
! Hdiaq(i,k,a,c) <--
! ( 2.00000000) D2(i,i,k,k) Y12(c,c)
! * Begin scaling analysis .... *
Declare Y12 as a tensor
for c1 in {core}:
 Read V2 from GA for c1
for c in {vir}:
 Read Hdiag from GA for c
  Hdiag_{(c)}(i, k, a) += 2 sum() D2(i,i,k,k) * Y12(c,c)
  Accumulate Hdiag_(c)(i,k,a) for c
! No.18
! Hdiag(i,k,a,c) <--
! ( -2.00000000) D2(i,k,k,i) Y13(a,c) kDelta(a,c)
! Kronecker's delta removed.
! * Begin scaling analysis .... *
Declare Y13 as a tensor
for c1 in {core}:
 Read V2 from GA for c1
for a in {vir}:
 Read Hdiag from GA for a
  Hdiag_(a)(i, k, a) += -2 sum() D2(i,k,k,i) * Y13(a,a)
  Accumulate Hdiag_(a)(i,k,a) for a
```

9 11, 12 16:46	eclipse_sort.dat	Page 11/145
!		
! No.19 ! Hdiag(i,k,a,c) < ! (-1.00000000) D2(i,i,k ! * Begin scaling analysis		
Declare Y14 as a tensor for c1 in {core}: Read V2 from GA for c1		
<pre>for c in {vir}: Read Hdiag from GA for c Hdiag_(c)(i, k, a) += su Accumulate Hdiag_(c)(i,k)</pre>	um() D2(i,i,k,k) * Y14(a,a) ,a) for c	
!		
! No.20 ! Hdiag(i,k,a,c) < ! (-1.00000000) D2(i,i,k ! * Begin scaling analysis		
Declare Y15 as a tensor for c1 in {core}: Read V2 from GA for c1		
<pre>for c in {vir}: Read Hdiag from GA for c Hdiag_(c)(i, k, a) += su Accumulate Hdiag_(c)(i,k)</pre>	um() D2(i,i,k,k) * Y15(c,c) ,a) for c	
!		
	<pre>x,k,o1,o3,o2,o4) V2(o1,o3,o2,o4) e rotated to match with each othe *</pre>	er.
<pre>for ol in {occ}: Read V2 from GA for ol for o3 in {occ}: for c in {vir}: Read Hdiag from GA for Read D4 from GA for OHdiag_(c)(i, k, a) += Accumulate Hdiag_(c)</pre>	o1, o3 = 0.5 sum(o2,o4) V2(,o3,o2,o4) *	* D4(,,i,i,k,k,o2,o4)
! !		
c) ! Kronecker's delta removed	c,i,o1,o3,o2,o4) V2(o1,o3,o2,o4) d. e rotated to match with each othe	
! * Begin scaling analysis for ol in {occ}: Read V2 from GA for ol for o3 in {occ}: for a in {vir}: Read Hdiag from GA for Read D4 from GA for	* or a	

9 11, 12 16:46	eclipse_sort.dat	Page 12/145
Accumulate Hdiag_(a)(i	,k,a) for a	
! No.23 ! Hdiag(i,k,a,c) < ! (2.00000000) D3(i,k,k, ! Kronecker's delta removed. ! Indices of ERI are rotated ! * Begin scaling analysis .	to match with LHS.	ta(a,c)
<pre>for a in {vir}: Read Hdiag from GA for a Read V2 from GA for a Hdiag_(a)(i, k, a) += 2 s Accumulate Hdiag_(a)(i,k,a</pre>	um(01,02) V2(,a,01,02) * D3) for a	(i,k,k,i,o1,o2)
!		
! No.24 ! Hdiag(i,k,a,c) < ! (1.00000000) D3(i,i,k, ! The indices of ERI are rot. ! * Begin scaling analysis .	ated to became virtual.	
<pre>for a in {vir}: Read V2 from GA for a for c in {vir}: Read Hdiag from GA for c Hdiag_(c)(i, k, a) += s Accumulate Hdiag_(c)(i,k)</pre>	um(o1,o2) V2(,a,o1,o2) * D3	(i,i,k,k,o1,o2)
!		
! No.25 ! Hdiag(i,k,a,c) < ! (1.00000000) D3(i,i,k, ! Indices of ERI are rotated ! * Begin scaling analysis .		
<pre>for c in {vir}: Read Hdiag from GA for c Read V2 from GA for c Hdiag_(c)(i, k, a) += sum Accumulate Hdiag_(c)(i,k,a</pre>	(o1,o2) V2(,c,o1,o2) * D3(i) for c	,i,k,k,o1,o2)
!		
! No.26 ! Hdiag(i,k,a,c) <	ol,o2,i) V2(ol,c,o2,a) kDelt	ta(a,c)
for a in {vir}: Read Hdiag from GA for a Read V2 from GA for a Hdiag_(a)(i, k, a) += 2 s Accumulate Hdiag_(a)(i,k,a	um(o1,o2) V2(,o1,o2,a) * D3) for a	(i,k,k,o1,o2,i)
! No.27		

```
eclipse_sort.dat
 9 11, 12 16:46
                                                                   Page 13/145
 Hdiaq(i,k,a,c) <--
     1.00000000) D3(i,o1,k,k,o2,i) V2(o1,a,o2,a)
! The indices of ERI are rotated to became virtual.
! * Begin scaling analysis .... *
for a in {vir}:
 Read V2 from GA for a
 for c in {vir}:
   Read Hdiag from GA for c
    Hdiag_{(c)(i, k, a)} += sum(o1,o2) V2(,o1,o2,a) * D3(i,o1,k,k,o2,i)
   Accumulate Hdiag_(c)(i,k,a) for c
! No.28
! Hdiag(i,k,a,c) <--
! ( 1.00000000) D3(i,i,k,o1,o2,k) V2(o1,c,o2,c)
! Indices of ERI are rotated to match with LHS.
! * Begin scaling analysis .... *
for c in {vir}:
 Read Hdiag from GA for c
 Read V2 from GA for c
 Hdiag_{(c)(i, k, a)} += sum(o1,o2) V2(,o1,o2,c) * D3(i,i,k,o1,o2,k)
 Accumulate Hdiag_(c)(i,k,a) for c
! No.29
! Hdiag(i,k,a,c) <--
! ( 1.00000000) D2(i,i,k,k) V2(a,a,c,c)
! Indices of ERI are rotated to match with LHS.
! * Begin scaling analysis .... *
for c in {vir}:
 Read Hdiag from GA for c
 Read V2 from GA for c
 Hdiag_(c)(i, k, a) += sum() V2(,c,a,a) * D2(i,i,k,k)
 Accumulate Hdiag_(c)(i,k,a) for c
! No.30
! Hdiag(i,k,a,c) <--
! ( 1.00000000) D2(i,k,k,i) V2(a,c,a,c)
! Indices of ERI are rotated to match with LHS.
! * Begin scaling analysis .... *
for c in {vir}:
 Read Hdiag from GA for c
 Read V2 from GA for c
 Hdiag_(c)(i, k, a) += sum() V2(,a,a,c) * D2(i,k,k,i)
 Accumulate Hdiag_(c)(i,k,a) for c
* 2 L:000V/R:000V
    0.50000000) V2(c1,c2,c3,c4) E5(c1,c2,i,k,m,c3,c4,m,k,i)
    0.50000000) V2(c1,c2,c3,c4) E4(c1,c2,i,k,c3,c4,i,k)
    -0.50000000) V2(c1,c2,c3,c4) E5(c1,c2,i,k,m,c3,c4,m,k,i)
    -0.50000000) V2(c1,c2,c3,c4) E4(c1,c2,i,k,c3,c4,i,k)
    0.50000000) V2(c1,o1,c2,o2) E5(c1,i,k,m,o1,c2,m,k,i,o2)
    0.50000000) V2(c1,o1,c2,o2) E4(c1,i,k,o1,c2,i,k,o2)
    0.50000000) V2(c1,m,c2,o1) E4(c1,i,k,m,c2,o1,k,i)
```

9 11, 12 16:46	eclipse_sort.dat	Page 14/145
	V2(c1,m,c2,o1) E4(c1,i,k,o1,c2,m,k,i)	
(0.50000000)	V2(c1,m,c2,m) E3(c1,i,k,c2,i,k) V2(c1,o1,c2,o2) E5(c1,i,k,m,o1,c2,m,k,i,o2)	
(-0.50000000)	V2(c1,01,c2,02) E3(c1,1,k,m,01,c2,m,k,1,02) V2(c1,01,c2,02) E4(c1,i,k,01,c2,i,k,02)	
(-0.50000000)	V2(c1,m,c2,o1) $E4(c1,i,k,m,c2,o1,k,i)$	
	V2(c1,i,c2,o1) E4(c1,i,k,m,c2,m,k,o1) V2(c1,i,c2,o1) E3(c1,i,k,c2,o1,k)	
(-0.50000000)	V2(c1,k,c2,o1) E3(c1,1,k,c2,o1,k) V2(c1,k,c2,o1) E4(c1,i,k,m,c2,m,o1,i)	
(-0.50000000)	V2(c1,k,c2,o1) E3(c1,i,k,c2,i,o1)	
(0.50000000)	V2(c1,c2,o2,o1) E5(c1,i,k,m,o1,o2,m,k,i,c2) V2(c1,c2,o2,o1) E4(c1,i,k,o1,o2,i,k,c2)	
(0.50000000)	V2(c1,c2,o1,m) E4(c1,i,k,m,o1,c2,k,i)	
	V2(c1,c2,m,o1) E4(c1,i,k,o1,i,m,k,c2)	
(0.50000000)	V2(c1,c2,m,m) E3(c1,i,k,i,c2,k) V2(c1,c2,o2,o1) E5(c1,i,k,m,o1,o2,m,k,i,c2)	
	V2(c1,c2,o2,o1) E4(c1,i,k,o1,o2,i,k,c2)	
(-0.50000000)	V2(c1,c2,o1,m) E4(c1,i,k,m,o1,c2,k,i)	
(-0.50000000)	V2(c1,c2,o1,i) E4(c1,i,k,m,o1,m,k,c2) V2(c1,c2,o1,i) E3(c1,i,k,o1,c2,k)	
(-0.50000000)	V2(c1,c2,o1,k) E4(c1,i,k,m,o1,m,c2,i)	
(-0.50000000)	V2(c1,c2,o1,k) E3(c1,i,k,o1,i,c2)	
(0.50000000)	V2(c1,a,c2,a) E4(c1,i,k,m,c2,m,k,i)	
(0.50000000)	V2(c1,a,c2,a) E3(c1,i,k,c2,i,k) V2(c1,c2,a,a) E4(c1,i,k,m,k,m,c2,i)	
(0.5000000)	V2(c1,c2,a,a) E3(c1,i,k,k,i,c2)	
	V2(c1,c2,o2,o1) E5(c1,i,k,m,o1,o2,m,k,i,c2)	
(0.50000000)	V2(c1,c2,o2,o1) E4(c1,i,k,o1,o2,i,k,c2) V2(c1,c2,o1,m) E4(c1,i,k,m,o1,c2,k,i)	
(0.50000000)	V2(c1,c2,m,o1) E4(c1,i,k,o1,i,m,k,c2)	
(0.50000000)	V2(c1,c2,m,m) E3(c1,i,k,i,c2,k)	
	V2(c1,c2,o2,o1) E5(c1,i,k,m,o1,o2,m,k,i,c2) V2(c1,c2,o2,o1) E4(c1,i,k,o1,o2,i,k,c2)	
	V2(c1,c2,o1,m) E4(c1,i,k,m,o1,c2,k,i)	
(-0.50000000)	V2(c1,c2,o1,i) $E4(c1,i,k,m,o1,m,k,c2)$	
(-0.50000000)	V2(c1,c2,o1,i) E3(c1,i,k,o1,c2,k) V2(c1,c2,o1,k) E4(c1,i,k,m,o1,m,c2,i)	
(-0.50000000)	V2(c1,c2,o1,k) E3(c1,i,k,o1,i,c2)	
(0.50000000)	V2(c1,o1,c2,o2) E5(c1,i,k,m,o1,c2,m,k,i,o2)	
(0.50000000)	V2(c1,o1,c2,o2) E4(c1,i,k,o1,c2,i,k,o2) V2(c1,m,c2,o1) E4(c1,i,k,m,c2,o1,k,i)	
(0.50000000)	V2(c1,m,c2,o1) E4(c1,i,k,o1,c2,m,k,i)	
(0.5000000)	V2(c1,m,c2,m) E3(c1,i,k,c2,i,k)	
	V2(c1,o1,c2,o2) E5(c1,i,k,m,o1,c2,m,k,i,o2) V2(c1,o1,c2,o2) E4(c1,i,k,o1,c2,i,k,o2)	
	V2(c1,01,c2,02) E4(c1,1,k,01,c2,1,k,02) V2(c1,m,c2,01) E4(c1,1,k,m,c2,01,k,i)	
(-0.50000000)	V2(c1,i,c2,o1) E4(c1,i,k,m,c2,m,k,o1)	
	V2(c1,i,c2,o1) E3(c1,i,k,c2,o1,k) V2(c1,k,c2,o1) E4(c1,i,k,m,c2,m,o1,i)	
	V2(c1,k,c2,o1) E3(c1,i,k,c2,i,o1)	
(0.5000000)	V2(o1,o2,o3,o4) E5(i,k,m,o1,o2,m,k,i,o3,o4)	
	V2(01,02,03,04) E4(i,k,01,02,i,k,03,04) V2(m,01,02,03) E4(i,k,m,01,02,k,i,03)	
	V2(m,o1,o2,o3) E4(i,k,m,o1,o3,k,i,o2)	
(0.5000000)	V2(m,o2,o1,o3) $E4(i,k,o1,o2,m,k,i,o3)$	
	V2(m,o1,m,o2) E3(i,k,o1,i,k,o2)	
	V2(m,m,o1,o2) E3(i,k,o1,o2,k,i) V2(m,o1,o2,o3) E4(i,k,o1,o2,m,k,o3,i)	
(0.5000000)	V2(m,m,o1,o2) E3(i,k,o1,o2,k,i)	
(0.50000000)	V2(m,o1,m,o2) E3(i,k,o1,i,k,o2)	
(-0.50000000)	V2(01,02,03,04) E5(i,k,m,01,02,m,k,i,03,04) V2(01,02,03,04) E4(i,k,01,02,i,k,03,04)	
(-0.50000000)	V2(m,o1,o2,o3) E4(i,k,m,o1,o2,k,i,o3)	
(-0.50000000)	V2(m,o1,o3,o2) E4(i,k,m,o1,o3,k,i,o2)	
	V2(i,o1,o2,o3) E4(i,k,m,o1,m,k,o2,o3) V2(i,o1,o2,o3) E3(i,k,o1,o2,k,o3)	
(-0.50000000)	V2(i,m,o1,o2) E3(i,k,m,o2,k,o1)	
(-0.50000000)	V2(i,o1,o3,o2) E4(i,k,m,o1,m,k,o3,o2)	
(-0.50000000) (-0.50000000)	V2(i,o1,o3,o2) E3(i,k,o1,o3,k,o2) V2(i,m,o2,o1) E3(i,k,m,o1,k,o2)	
1	. , , ,,,,,,,,,	

```
eclipse_sort.dat
 9 11, 12 16:46
                                                                       Page 15/145
    -0.50000000) V2(k,o1,o2,o3) E4(i,k,m,o1,m,o2,i,o3)
    -0.50000000) V2(k,o1,o2,o3) E3(i,k,o1,i,o2,o3)
    -0.50000000) V2(k,m,o1,o2) E3(i,k,m,o2,o1,i)
    -0.50000000) V2(k,o1,o3,o2) E4(i,k,m,o1,m,o3,i,o2)
    -0.50000000) V2(k,o1,o3,o2) E3(i,k,o1,i,o3,o2)
    -0.50000000) V2(k,m,o2,o1) E3(i,k,m,o1,o2,i)
    -0.50000000) V2(i,k,o1,o2) E3(i,k,m,m,o2,o1)
    -0.50000000) V2(i,k,o1,o2) E2(i,k,o1,o2)
    -0.50000000) V2(i,k,o2,o1) E3(i,k,m,m,o1,o2)
    -0.50000000) V2(i,k,o2,o1) E2(i,k,o2,o1)
     0.50000000) V2(o1,a,o2,a) E4(i,k,m,o1,m,k,i,o2)
     0.50000000) V2(o1,a,o2,a) E3(i,k,o1,i,k,o2)
     0.50000000) V2(m,a,o1,a) E3(i,k,m,o1,k,i) 0.50000000) V2(m,a,o1,a) E3(i,k,o1,m,k,i)
     0.50000000) V2(m,a,m,a) E2(i,k,i,k)
     0.50000000) V2(o1,o2,a,a) E4(i,k,m,o1,m,o2,i,k)
     0.50000000) V2(o1,o2,a,a) E3(i,k,o1,i,o2,k)
     0.50000000) V2(m,o1,a,a) E3(i,k,m,k,o1,i)
     0.50000000) V2(m,o1,a,a) E3(i,k,o1,m,i,k)
     0.50000000) V2(m,m,a,a) E2(i,k,k,i)
     0.50000000) V2(c1,c2,a,a) E4(c1,i,k,m,k,m,c2,i)
     0.50000000) V2(c1,c2,a,a) E3(c1,i,k,k,i,c2)
     0.50000000) V2(c1,a,c2,a) E4(c1,i,k,m,c2,m,k,i)
     0.50000000) V2(c1,a,c2,a) E3(c1,i,k,c2,i,k)
     0.50000000) V2(o1,o2,a,a) E4(i,k,m,o1,m,o2,i,k)
0.50000000) V2(o1,o2,a,a) E3(i,k,o1,i,o2,k)
     0.50000000) V2(m,o1,a,a) E3(i,k,m,k,o1,i)
     0.50000000) V2(m,o1,a,a) E3(i,k,o1,m,i,k)
     0.50000000) V2(m,m,a,a) E2(i,k,k,i)
     0.50000000) V2(o1,a,o2,a) E4(i,k,m,o1,m,k,i,o2)
     0.50000000) V2(o1,a,o2,a) E3(i,k,o1,i,k,o2)
     0.50000000) V2(m,a,o1,a) E3(i,k,m,o1,k,i)
     0.50000000) V2(m,a,o1,a) E3(i,k,o1,m,k,i)
     0.50000000) V2(m,a,m,a) E2(i,k,i,k)
1.00000000) Ecas E3(i,k,m,m,k,i)
     1.00000000) Ecas E2(i,k,i,k)
Decompose RDMs .....
< RESULT >
    0: (
             1.00000000) D3(i,k,m,o1,k,i) h(m,o1)
            1.00000000) D2(i,k,i,k) h(m,m)
    2: (
            -1.00000000) D3(i,k,m,m,k,o1) h(i,o1)
            -1.00000000) D2(i,k,o1,k) h(i,o1)
    3: (
    4: (
            -1.000000000) D3(i,k,m,m,o1,i) h(k,o1)
    5: (
            -1.00000000) D2(i,k,i,o1) h(k,o1)
    6: (
            1.00000000) D3(i,k,m,m,k,i) h(a,a)
    7: (
             1.00000000) D2(i,k,i,k) h(a,a)
    8: (
             2.00000000) D3(i,k,m,o1,k,i) V2(c1,m,c1,o1)
             2.00000000) D2(i,k,i,k) V2(c1,m,c1,m)
    9: (
  10: (
            -2.00000000) D3(i,k,m,m,k,o1) V2(c1,i,c1,o1)
  11: (
            -2.00000000) D2(i,k,o1,k) V2(c1,i,c1,o1)
  12 : (
            -2.00000000) D3(i,k,m,m,o1,i) V2(c1,k,c1,o1)
            -2.00000000) D2(i,k,i,o1) V2(c1,k,c1,o1)
  14: (
            -1.00000000) D3(i,k,m,o1,k,i) V2(c1,c1,m,o1)
            -1.00000000) D2(i,k,i,k) V2(c1,c1,m,m)
  15: (
  16: (
             1.00000000) D3(i,k,m,m,k,o1) V2(c1,c1,i,o1)
  17: (
             1.00000000) D2(i,k,o1,k) V2(c1,c1,i,o1)
             1.00000000) D3(i,k,m,m,o1,i) V2(c1,c1,k,o1)
  18: (
  19: (
             1.00000000) D2(i,k,i,o1) V2(c1,c1,k,o1)
  20: (
             2.000000000) D3(i,k,m,m,k,i) V2(c1,a,c1,a)
             2.00000000) D2(i,k,i,k) V2(c1,a,c1,a)
  21: (
  22: (
            -1.00000000) D3(i,k,m,m,k,i) V2(c1,c1,a,a)
            -1.00000000) D2(i,k,i,k) V2(c1,c1,a,a)
             1.00000000) D4(i,k,m,o3,o2,k,i,o1) V2(m,o3,o2,o1)
  24: (
  25 : (
             1.00000000) D3(i,k,o2,i,k,o1) V2(m,o2,m,o1)
             1.00000000) D3(i,k,o2,o1,k,i) V2(m,m,o2,o1)
            -1.00000000) D4(i,k,m,o3,m,k,o2,o1) V2(i,o3,o2,o1)
```

9 11, 12 16:46	eclipse_sort.dat	Page 16/145
28 : (-1.00000000 29 : (-1.00000000 30 : (-1.00000000 31 : (-1.00000000 32 : (-1.00000000 33 : (-1.00000000 34 : (-1.00000000 35 : (1.00000000 36 : (1.00000000 37 : (2.00000000 38 : (1.00000000 40 : (1.00000000 41 : (2.00000000 43 : (1.00000000000000000000000000000000000) D3(i,k,o3,o2,k,o1) V2(i,o3,o2,o1)) D3(i,k,m,o2,k,o1) V2(i,m,o1,o2)) D4(i,k,m,o3,m,o2,i,o1) V2(k,o3,o2,o1)) D3(i,k,o3,i,o2,o1) V2(k,o3,o2,o1)) D3(i,k,m,n2,o1,i) V2(k,m,o1,o2)) D3(i,k,m,m,o2,o1) V2(i,k,o1,o2)) D2(i,k,o2,o1) V2(i,k,o2,o1)) D4(i,k,m,o1,m,k,i,o2) V2(o1,a,o2,a)) D3(i,k,o2,i,k,o1) V2(o2,a,o1,a)) D3(i,k,o2,i,k,o1) V2(m,a,o1,a)) D3(i,k,m,o1,m,k,i) V2(m,a,o1,a)) D4(i,k,m,o1,m,o2,i,k) V2(o1,o2,a,a)) D4(i,k,m,o1,m,o2,i,k) V2(o1,o2,a,a)) D3(i,k,o2,i,o1,k) V2(o2,o1,a,a)) D3(i,k,o2,i,o1,k) V2(m,o1,a,a)) D3(i,k,o2,i,o1,k) V2(m,o1,a,a)) D3(i,k,k,i) V2(m,m,a,a)) Ecas D3(i,k,m,m,k,i)) Ecas D2(i,k,i,k)	
1 : (1.00000000) D3(i,m,k,k,01,i) h(m,01)) D2(i,i,k,k) h(m,m)) D3(i,m,k,k,m,01) h(i,01)) D2(i,01,k,k) h(i,01)) D3(i,m,k,01,m,i) h(k,01)) D3(i,m,k,k,m,i) h(a,a)) D3(i,m,k,k,01,i) V2(c1,c1,m,01)) D3(i,m,k,k,m,01) V2(c1,c1,i,01)) D2(i,i,k,k) V2(c1,c1,i,01)) D3(i,m,k,k,m,01) V2(c1,c1,i,01)) D2(i,i,k,k) V2(c1,c1,i,01)) D3(i,m,k,k,m,01) V2(c1,c1,k,01)) D3(i,m,k,k,01,i) V2(c1,c1,k,01)) D3(i,m,k,k,01,i) V2(c1,c1,k,01)) D3(i,m,k,k,01,i) V2(c1,m,c1,m)) D3(i,m,k,k,m,01) V2(c1,i,c1,01)) D2(i,i,k,k) V2(c1,i,c1,01)) D2(i,i,k,k) V2(c1,i,c1,01)) D3(i,m,k,k,m,i) V2(c1,k,c1,01)) D3(i,m,k,k,m,i) V2(c1,k,c1,01)) D3(i,m,k,k,m,i) V2(c1,c1,a,a)) D2(i,i,k,k) V2(c1,c1,a,a)) D3(i,m,k,k,m,i) V2(c1,a,c1,a)) D4(i,i,k,k) V2(c1,a,c1,a)) D4(i,i,k,k) V2(c1,a,c1,a)) D4(i,i,k,k) V2(c1,a,c1,a)) D4(i,i,k,k,01,03,02,i) V2(m,02,01,03)) D3(i,i,k,k,01,02) V2(m,m,01,02)) D4(i,m,k,k,m,01) V2(i,02,01,03)) D3(i,02,k,k,m,01) V2(i,02,01,03)) D3(i,02,k,k,m,01) V2(i,02,01,03)) D3(i,02,k,k,m,01) V2(i,02,01,03)) D3(i,i,k,02,03,01) V2(k,02,01,03)) D3(i,i,k,02,03,01) V2(k,02,01,03)) D3(i,i,k,02,03,01) V2(k,02,01,03)) D3(i,i,k,02,03,01) V2(k,02,01,03)) D3(i,i,k,02,03,01) V2(k,02,01,03)) D3(i,i,k,02,03,01) V2(k,02,01,03)) D3(i,i,k,02,m,01) V2(i,02,a,a)) D3(i,i,k,01,02) V2(o1,a,a)) D3(i,i,k,01,02,k) V2(o1,a,02,a)) D3(i,i,k,01,02,k) V2(o1,a,02,a)) D3(i,k,k,01,m,i) V2(m,a,01,a)) D2(i,k,k,i) V2(m,a,m,a)) Ecas D3(i,m,k,k,m,i) Ecas D2(i,i,k,k)	
) D3(i,m,k,k,o1,i) h(m,o1)) D2(i,i,k,k) h(m,m)	

	:46	eclip	se_sort.c	lat		Pa	ige 17	/145
2 : (3 : (4 : (5 : (6 : (7 : (8 : (9 : (10 : (11 : (12 : (13 : (14 : (15 : (16 : (17 : (18 : (19 : (20 : (21 : (22 : (24 : (25 : (28 : (29 : (28 : (29 : (30 : (31 : (32 : (33 : (33 : (33 : (33 : (33 : (33 : (33 : (33 : (33 : (33 : (33 : (33 : (33 : (33 : (33 : (34 : (40 : (41 : (42 : (44 : (etting up for a contained of a contained up for a c	-1.00000000) -1.00000000) -1.00000000) -1.00000000) -1.00000000) -1.00000000) -2.00000000) -2.00000000) -2.00000000) -1.00000000)	D3(i,m,k,k,m, D2(i,o1,k,k) D3(i,m,k,o1,n D2(i,i,k,o1) D3(i,m,k,k,m, D2(i,i,k,k) D3(i,m,k,k,m, D2(i,i,k,k) D3(i,m,k,k,m, D2(i,i,k,k) D3(i,m,k,k,n,n D2(i,i,k,k) D3(i,m,k,c),n D2(i,i,k,k) D3(i,m,k,c),n D2(i,i,k,k) D3(i,m,k,k,m,n D3(i,i,k,k,c) D3(i,i,k,k,c) D3(i,i,k,k,c,n,n D3(i,i,k,k,c,n,n,n D3(i,i,k,k,c,n,n,n D3(i,i,k,k,c,n,n,n,n D3(i,i,k,k,c,n,n,n,n,n,n,n,n,n,n,n,n,n,n,n,n,n	o1) h(i,o) h(i,o) h(i,o1) h,i) h(k,o) h(k,o1) i) h(a,a) h(a,a) h(a,a) v2(c1,c1,m o1) V2(c1,c1,d n,i) V2(c1,c1,d n,i) V2(c1,c1,d n,i) V2(c1,c1,d n,i) V2(c1,d,d n,i) V2(c1,d n,i) V2(m n,i)	(c1,m,o1) (m) (c1,i,o1) (c1,i,o2) (c1,i,o2,o1) (c1,i,o2,o1) (c1,i,o2,o1) (c1,i,o2,o1) (c1,i,o2,o1) (c1,i,o2,o1) (c1,i,o2,o1) (c1,i,o2,o1) (c1,i,o2,o1) (c1,i,o2,o1,o2) (c1,i,o2,o1,o2) (c1,i,o2,o1,o2) (c1,i,o2,o1,o2) (c1,i,o2,o1,o2) (c1,i,o2)	,03) ,03) a)			
8 888888888 8880.	8 8 8 8 8 8 8 8 8 8	8888	,8.	,8. 8	888888		88888	,088
8 8888	8 8888		,888.	,888.		8888		8888
8 8888 8	8 8888		. `8888.	. `8888.		8888		8888
8 8888 , 8p	8 8888		8. `8888.			8888		8888
88	8888 8 888888		3′8.`8888,8			8888		8888
8 8888	8 8888			' '8.'8888.		8888		8888
8 8888 ,8P	8 8888	,8′		`8.`8888		8888		8888
8 8888 ,8P	8 8888	,8′		`8.`888		8888		8888
8 8888 ,88'	8 8888	,8′	`8	`8.`88		8888	`	8888
, 00	0 000000	888888 ,8'	`	`8.`8	888. 8	8888		1888

```
eclipse sort.dat
  9 11, 12 16:46
                                                                     Page 18/145
The linked formulas ....
         1.00000000) D3(i,m,k,k,o1,i) h(m,o1)
         1.000000000) D2(i,i,k,k) h(m,m)
2:
        -1.00000000) D3(i,m,k,k,m,o1) h(i,o1)
3 :
        -1.00000000) D2(i,o1,k,k) h(i,o1)
        -1.00000000) D3(i,m,k,o1,m,i) h(k,o1)
5:
        -1.00000000) D2(i,i,k,o1) h(k,o1)
6:
         1.00000000) D3(i,m,k,k,m,i) h(a,a)
7:
         1.00000000) D2(i,i,k,k) h(a,a)
8 :
         2.00000000) D3(i,m,k,k,o1,i) Y0(m,o1)
9: (
         2.00000000) D2(i,i,k,k) Y1(m,m)
10:
         -2.00000000) D3(i,m,k,k,m,o1) Y2(i,o1)
11: (
         -2.00000000) D2(i,o1,k,k) Y3(i,o1)
12:
         -2.00000000) D3(i,m,k,o1,m,i) Y4(k,o1)
13
         -2.00000000) D2(i,i,k,o1) Y5(k,o1)
         -1.00000000) D3(i,m,k,k,o1,i) Y6(m,o1)
14 :
15: (
         -1.00000000) D2(i,i,k,k) Y7(m,m)
16:
          1.00000000) D3(i,m,k,k,m,o1) Y8(i,o1)
17 :
          1.00000000) D2(i,o1,k,k) Y9(i,o1)
18 :
          1.00000000) D3(i,m,k,o1,m,i) Y10(k,o1)
19
          1.00000000) D2(i,i,k,o1) Y11(k,o1)
20:
          2.00000000) D3(i,m,k,k,m,i) Y12(a,a)
21 :
          2.00000000) D2(i,i,k,k) Y13(a,a)
22 :
         -1.00000000) D3(i,m,k,k,m,i) Y14(a,a)
23 :
         -1.000000000 D2(i,i,k,k) Y15(a,a)
24:
          1.00000000) D4(i,m,k,k,o1,o3,o2,i) V2(m,o2,o1,o3)
25
          1.00000000) D3(i,i,k,k,o1,o2) V2(m,m,o1,o2)
1.00000000) D3(i,o1,k,k,o2,i) V2(m,o1,m,o2)
26
2.7 :
         -1.00000000) D4(i,m,k,k,m,o2,o3,o1) V2(i,o2,o1,o3)
28 :
         -1.00000000) D3(i,o2,k,k,o3,o1) V2(i,o2,o1,o3)
29:
         -1.00000000) D3(i,o2,k,k,m,o1) V2(i,o1,m,o2)
30 :
         -1.00000000) D4(i,m,k,o2,m,i,o3,o1) V2(k,o2,o1,o3)
31 :
         -1.00000000) D3(i,i,k,o2,o3,o1) V2(k,o2,o1,o3)
32:
         -1.00000000) D3(i,m,o1,k,o2,i) V2(k,o1,m,o2)
         -1.00000000) D3(i,m,k,o2,m,o1) V2(i,o1,k,o2)
33:
34 :
         -1.00000000) D2(i,o2,k,o1) V2(i,o2,k,o1)
35 :
          1.00000000) D4(i,m,k,k,m,i,o1,o2) V2(o1,o2,a,a)
          1.00000000) D3(i,i,k,k,o1,o2) V2(o1,o2,a,a)
36: (
37
          2.00000000) D3(i,m,k,k,o1,i) V2(m,o1,a,a)
38
          1.00000000) D2(i,i,k,k) V2(m,m,a,a)
39
          1.00000000) D4(i,m,k,o1,m,i,o2,k) V2(o1,a,o2,a)
          1.00000000) D3(i,i,k,o1,o2,k) V2(o1,a,o2,a)
41 :
          2.00000000) D3(i,k,k,o1,m,i) V2(m,a,o1,a)
42 : (
          1.00000000) D2(i,k,k,i) V2(m,a,m,a)
43
          1.00000000) Ecas D3(i,m,k,k,m,i)
          1.00000000) Ecas D2(i,i,k,k)
The content of each effective tensor ....
Y0 <--
            1.00000000) V2(c1,c1,m,o1)
Y1 <--
            1.00000000) V2(c1,c1,m,m)
Y2 <--
            1.00000000)
                         V2(c1,c1,i,o1)
Y3 <--
            1.00000000)
                         V2(c1,c1,i,o1)
Y4 <--
            1.00000000)
                         V2(c1,c1,k,o1)
Y5 <--
            1.00000000)
                         V2(c1,c1,k,o1)
Y6 <--
            1.00000000)
                         V2(c1,m,c1,o1)
Y7 <--
            1.00000000)
                         V2(c1,m,c1,m)
Y8 <--
            1.00000000)
                         V2(c1,i,c1,o1)
Y9 <-- (
            1.00000000)
                         V2(c1,i,c1,o1)
Y10 <--
             1.00000000) V2(c1,k,c1,o1
Y11 <--
             1.00000000) V2(c1,k,c1,o1)
Y12 <--
             1.00000000) V2(c1,c1,a,a)
Y13 <--
             1.00000000) V2(c1,c1,a,a)
Y14 <--
             1.00000000)
                         V2(c1,a,c1,a)
Y15 <-- (
             1.00000000) V2(c1,a,c1,a)
! No.0
! Hdiag(i,k,m,a) <--
```

```
eclipse_sort.dat
                                                                    Page 19/145
 9 11, 12 16:46
      1.00000000) D3(i,m,k,k,o1,i) h(m,o1)
! * Begin scaling analysis .... '
for a in {vir}:
 Read Hdiag from GA for a
 Hdiag_{(a)}(i, k, m) += sum(o1) D3(i,m,k,k,o1,i) * h(m,o1)
 Accumulate Hdiag (a)(i,k,m) for a
! No.1
! Hdiaq(i,k,m,a) <--
! ( 1.00000000) D2(i,i,k,k) h(m,m)
! * Begin scaling analysis .... *
for a in {vir}:
 Read Hdiag from GA for a
 Hdiag_(a)(i, k, m) += sum() D2(i,i,k,k) * h(m,m)
 Accumulate Hdiag_(a)(i,k,m) for a
! Hdiag(i,k,m,a) <--
! ( -1.00000000) D3(i,m,k,k,m,o1) h(i,o1)
! * Begin scaling analysis .... *
for a in {vir}:
 Read Hdiag from GA for a
 Hdiag_(a)(i, k, m) += sum(o1) D3(i, m, k, k, m, o1) * h(i, o1)
 Accumulate Hdiag_(a)(i,k,m) for a
! Hdiag(i,k,m,a) <--
! ( -1.00000000) D2(i,o1,k,k) h(i,o1)
! * Begin scaling analysis .... *
for a in {vir}:
 Read Hdiag from GA for a
 Hdiag_{(a)}(i, k, m) += sum(o1) D2(i,o1,k,k) * h(i,o1)
 Accumulate Hdiag_(a)(i,k,m) for a
! Hdiag(i,k,m,a) <--
! (-1.00000000) D3(i,m,k,o1,m,i) h(k,o1)
! * Begin scaling analysis .... *
for a in {vir}:
 Read Hdiag from GA for a
 Hdiag_{(a)}(i, k, m) += sum(o1) D3(i, m, k, o1, m, i) * h(k, o1)
 Accumulate Hdiag_(a)(i,k,m) for a
! No.5
! Hdiag(i,k,m,a) <--
! ( -1.00000000) D2(i,i,k,o1) h(k,o1)
! * Begin scaling analysis .... *
for a in {vir}:
```

```
eclipse_sort.dat
 9 11, 12 16:46
                                                                     Page 20/145
  Read Hdiag from GA for a
  Hdiag_(a)(i, k, m) += sum(o1) D2(i,i,k,o1) * h(k,o1)
  Accumulate Hdiag (a)(i,k,m) for a
! No.6
! Hdiag(i,k,m,a) <--
! ( 1.00000000) D3(i,m,k,k,m,i) h(a,a)
! * Begin scaling analysis .... *
for a in {vir}:
 Read Hdiag from GA for a
  Hdiag_(a)(i, k, m) += sum() D3(i,m,k,k,m,i) * h(a,a)
  Accumulate Hdiag (a)(i,k,m) for a
1 No 7
! Hdiag(i,k,m,a) <--
! ( 1.00000000) D2(i,i,k,k) h(a,a)
! * Begin scaling analysis .... *
for a in {vir}:
 Read Hdiag from GA for a
 Hdiag_{(a)}(i, k, m) += sum() D2(i,i,k,k) * h(a,a)
Accumulate Hdiag_{(a)}(i,k,m) for a
! Hdiaq(i,k,m,a) <--
! ( 2.00000000) D3(i,m,k,k,o1,i) Y0(m,o1)
! * Begin scaling analysis .... *
Declare Y0 as a tensor
for c1 in {core}:
 Read V2 from GA for c1
for a in {vir}:
 Read Hdiag from GA for a
  Hdiag_{(i)}(i, k, m) += 2 sum(o1) D3(i, m, k, k, o1, i) * Y0(m, o1)
  Accumulate Hdiag_(a)(i,k,m) for a
! No.9
! Hdiag(i,k,m,a) <--
! ( 2.00000000) D2(i,i,k,k) Y1(m,m)
! * Begin scaling analysis .... *
Declare Y1 as a tensor
for c1 in {core}:
 Read V2 from GA for c1
for a in {vir}:
 Read Hdiag from GA for a
 Hdiag_{(a)}(i, k, m) += 2 sum() D2(i,i,k,k) * Y1(m,m)
 Accumulate Hdiag_(a)(i,k,m) for a
! No.10
! Hdiag(i,k,m,a) <--
```

```
eclipse_sort.dat
 9 11, 12 16:46
                                                                    Page 21/145
! (-2.00000000) D3(i,m,k,k,m,o1) Y2(i,o1)
! * Begin scaling analysis .... '
Declare Y2 as a tensor
for c1 in {core}:
 Read V2 from GA for c1
for a in {vir}:
 Read Hdiag from GA for a
 Hdiag_{(a)}(i, k, m) += -2 sum(o1) D3(i,m,k,k,m,o1) * Y2(i,o1)
 Accumulate Hdiag (a)(i,k,m) for a
! No.11
! Hdiag(i,k,m,a) <--
! ( -2.00000000) D2(i,o1,k,k) Y3(i,o1)
! * Begin scaling analysis .... *
Declare Y3 as a tensor
for c1 in {core}:
 Read V2 from GA for c1
for a in {vir}:
 Read Hdiag from GA for a
 Hdiag_(a)(i, k, m) += -2 sum(o1) D2(i,o1,k,k) * Y3(i,o1)
 Accumulate Hdiag (a)(i,k,m) for a
! No.12
! Hdiaq(i,k,m,a) <--
! (-2.00000000) D3(i,m,k,o1,m,i) Y4(k,o1)
! * Begin scaling analysis .... *
Declare Y4 as a tensor
for c1 in {core}:
Read V2 from GA for c1
for a in {vir}:
 Read Hdiag from GA for a
 Hdiag_{(a)}(i, k, m) += -2 sum(o1) D3(i, m, k, o1, m, i) * Y4(k, o1)
 Accumulate Hdiag_(a)(i,k,m) for a
! No.13
! Hdiag(i,k,m,a) <--
! ( -2.00000000) D2(i,i,k,o1) Y5(k,o1)
! * Begin scaling analysis .... *
Declare Y5 as a tensor
for c1 in {core}:
 Read V2 from GA for c1
for a in {vir}:
 Read Hdiag from GA for a
 Hdiag_{(a)}(i, k, m) += -2 sum(o1) D2(i,i,k,o1) * Y5(k,o1)
 Accumulate Hdiag_(a)(i,k,m) for a
! No.14
! Hdiag(i,k,m,a) <--
! (-1.00000000) D3(i,m,k,k,o1,i) Y6(m,o1)
```

```
eclipse sort.dat
  9 11, 12 16:46
                                                                             Page 22/145
! * Begin scaling analysis .... *
Declare Y6 as a tensor
for c1 in {core}:
 Read V2 from GA for c1
for a in {vir}:
  Read Hdiag from GA for a
  \begin{array}{lll} \mbox{Hdiag}_{-}(a) \mbox{ii}, \ k, \ m) \ += \ \mbox{sum}(ol) \ \mbox{D3}(i, m, k, k, ol, i) \ * \ Y6(m, ol) \\ \mbox{Accumulate Hdiag}_{-}(a) (i, k, m) \ \mbox{for a} \end{array}
! No.15
! Hdiaq(i,k,m,a) <--
! ( -1.00000000) D2(i,i,k,k) Y7(m,m)
! * Begin scaling analysis .... *
Declare Y7 as a tensor
for c1 in {core}:
   Read V2 from GA for c1
for a in {vir}:
  Read Hdiag from GA for a
  Hdiag_(a)(i, k, m) += sum() D2(i,i,k,k) * Y7(m,m)
  Accumulate Hdiag_(a)(i,k,m) for a
! Hdiag(i,k,m,a) <--
! ( 1.00000000) D3(i,m,k,k,m,o1) Y8(i,o1)
! * Begin scaling analysis .... '
Declare Y8 as a tensor
for c1 in {core}:
Read V2 from GA for c1
for a in {vir}:
 Read Hdiag from GA for a
  Hdiag_{(a)}(i, k, m) += sum(o1) D3(i, m, k, k, m, o1) * Y8(i, o1)
  Accumulate Hdiag_(a)(i,k,m) for a
! Hdiag(i,k,m,a) <--
! ( 1.00000000) D2(i,o1,k,k) Y9(i,o1)
! * Begin scaling analysis .... *
Declare Y9 as a tensor
for c1 in {core}:
 Read V2 from GA for cl
for a in {vir}:
  Read Hdiag from GA for a
  Hdiag_{(a)}(i, k, m) += sum(o1) D2(i,o1,k,k) * Y9(i,o1)
  Accumulate Hdiag_(a)(i,k,m) for a
! No.18
! Hdiag(i,k,m,a) <--
! ( 1.00000000) D3(i,m,k,o1,m,i) Y10(k,o1)
! * Begin scaling analysis .... *
```

```
eclipse_sort.dat
 9 11, 12 16:46
                                                                   Page 23/145
Declare Y10 as a tensor
for c1 in {core}:
 Read V2 from GA for c1
for a in {vir}:
 Read Hdiag from GA for a
 Hdiag_(a)(i, k, m) += sum(o1) D3(i,m,k,o1,m,i) * Y10(k,o1)
 Accumulate Hdiag_(a)(i,k,m) for a
! No.19
! Hdiag(i,k,m,a) <--
! ( 1.00000000) D2(i,i,k,o1) Y11(k,o1)
! * Begin scaling analysis .... *
Declare Y11 as a tensor
for c1 in {core}:
 Read V2 from GA for c1
for a in {vir}:
 Read Hdiag from GA for a
 Hdiag_(a)(i, k, m) += sum(o1) D2(i,i,k,o1) * Y11(k,o1)
 Accumulate Hdiag_(a)(i,k,m) for a
! No.20
! Hdiag(i,k,m,a) <--
! ( 2.00000000) D3(i,m,k,k,m,i) Y12(a,a)
! * Begin scaling analysis .... *
Declare Y12 as a tensor
for c1 in {core}:
 Read V2 from GA for c1
for a in {vir}:
 Read Hdiag from GA for a
 Hdiag_{(a)}(i, k, m) += 2 sum() D3(i,m,k,k,m,i) * Y12(a,a)
 Accumulate Hdiag_(a)(i,k,m) for a
! No.21
! Hdiag(i,k,m,a) <--
! ( 2.00000000) D2(i,i,k,k) Y13(a,a)
! * Begin scaling analysis .... *
Declare Y13 as a tensor
for c1 in {core}:
 Read V2 from GA for c1
for a in {vir}:
 Read Hdiag from GA for a
 Hdiag_{(a)}(i, k, m) += 2 sum() D2(i,i,k,k) * Y13(a,a)
 Accumulate Hdiag_(a)(i,k,m) for a
! No.22
! Hdiag(i,k,m,a) <--
! ( -1.00000000) D3(i,m,k,k,m,i) Y14(a,a)
! * Begin scaling analysis .... *
```

```
eclipse sort.dat
  9 11, 12 16:46
                                                                   Page 24/145
Declare Y14 as a tensor
for c1 in {core}:
 Read V2 from GA for c1
for a in {vir}:
 Read Hdiag from GA for a
  Hdiag(a)(i, k, m) += sum() D3(i, m, k, k, m, i) * Y14(a, a)
  Accumulate Hdiag_(a)(i,k,m) for a
! Hdiaq(i,k,m,a) <--
! ( -1.00000000) D2(i,i,k,k) Y15(a,a)
! * Begin scaling analysis .... *
Declare Y15 as a tensor
for c1 in {core}:
 Read V2 from GA for c1
for a in {vir}:
 Read Hdiag from GA for a
 Hdiag_{(a)}(i, k, m) += sum() D2(i,i,k,k) * Y15(a,a)
  Accumulate Hdiag_(a)(i,k,m) for a
! Hdiaq(i,k,m,a) <--
! ( 1.00000000) D4(i,m,k,k,o1,o3,o2,i) V2(m,o2,o1,o3)
! Indices of ERI and D4 are rotated to match with each other.
! * Begin scaling analysis .... *
for m in {occ}:
 Read V2 from GA for m
  for a in {vir}:
    Read Hdiag from GA for a
    for i in {occ}:
     Read D4 from GA for m, i
     Hdiag_{(a)}(i, k, m) += sum(o2,o1,o3) V2(,o2,o1,o3) * D4(,,k,k,o3,o1,i,o2)
   Accumulate Hdiag (a)(i,k,m) for a
! No.25
! Hdiag(i,k,m,a) <--
! ( 1.00000000) D3(i,i,k,k,o1,o2) V2(m,m,o1,o2)
! * Begin scaling analysis .... *
for m in {occ}:
 Read V2 from GA for m
  for a in {vir}:
   Read Hdiag from GA for a
   Hdiag_{(a)}(i, k, m) += sum(o1,o2) V2(,m,o1,o2) * D3(i,i,k,k,o1,o2)
   Accumulate Hdiag_(a)(i,k,m) for a
1 No. 26
! Hdiag(i,k,m,a) <--
! ( 1.00000000) D3(i,o1,k,k,o2,i) V2(m,o1,m,o2)
! * Begin scaling analysis .... *
for m in {occ}:
 Read V2 from GA for m
```

```
eclipse_sort.dat
 9 11, 12 16:46
                                                                   Page 25/145
 for a in {vir}:
    Read Hdiag from GA for a
    Hdiag_{(a)(i, k, m)} += sum(o1,o2) V2(,o1,m,o2) * D3(i,o1,k,k,o2,i)
   Accumulate Hdiag (a)(i,k,m) for a
! No.27
! Hdiaq(i,k,m,a) <--
! ( -1.00000000) D4(i,m,k,k,m,o2,o3,o1) V2(i,o2,o1,o3)
! Indices of ERI and D4 are rotated to match with each other.
! * Begin scaling analysis .... *
for i in {occ}:
 Read V2 from GA for i
 for m in {occ}:
   for a in {vir}:
     Read Hdiag from GA for a
     Read D4 from GA for i, m
     Hdiag_{(a)}(i, k, m) += sum(02,01,03) V2(,02,01,03) * D4(,,k,k,m,02,03,01)
     Accumulate Hdiag_(a)(i,k,m) for a
! No.28
! Hdiaq(i,k,m,a) <--
! ( -1.00000000) D3(i,o2,k,k,o3,o1) V2(i,o2,o1,o3)
! * Begin scaling analysis .... *
for i in {occ}:
 Read V2 from GA for i
 for a in {vir}:
   Read Hdiag from GA for a
   Hdiag_{(a)}(i, k, m) += sum(02,01,03) V2(,02,01,03) * D3(i,02,k,k,03,01)
   Accumulate Hdiag (a)(i,k,m) for a
1 No. 29
! Hdiag(i,k,m,a) <--
! (-1.00000000) D3(i,o2,k,k,m,o1) V2(i,o1,m,o2)
! * Begin scaling analysis .... *
for i in {occ}:
 Read V2 from GA for i
 for a in {vir}:
   Read Hdiag from GA for a
   Hdiag_{(a)}(i, k, m) += sum(o1,o2) V2(,o1,m,o2) * D3(i,o2,k,k,m,o1)
   Accumulate Hdiag_(a)(i,k,m) for a
! No.30
! Hdiag(i,k,m,a) <--
! (-1.00000000) D4(i,m,k,o2,m,i,o3,o1) V2(k,o2,o1,o3)
! Indices of ERI and D4 are rotated to match with each other.
! * Begin scaling analysis .... *
for k in {occ}:
 Read V2 from GA for k
 for o2 in {occ}:
   for a in {vir}:
     Read Hdiag from GA for a
     Read D4 from GA for k, o2
     Hdiag_{(a)}(i, k, m) += sum(o1,o3) V2(,o2,o1,o3) * D4(,,i,m,m,i,o3,o1)
```

```
eclipse_sort.dat
  9 11, 12 16:46
                                                                   Page 26/145
      Accumulate Hdiag (a)(i,k,m) for a
! Hdiaq(i,k,m,a) <--
! (-1.00000000) D3(i,i,k,o2,o3,o1) V2(k,o2,o1,o3)
! * Begin scaling analysis .... *
for k in {occ}:
 Read V2 from GA for k
  for a in {vir}:
    Read Hdiag from GA for a
    Hdiag_{(a)}(i, k, m) += sum(02,01,03) V2(,02,01,03) * D3(i,i,k,02,03,01)
    Accumulate Hdiag (a)(i,k,m) for a
1 No 32
! Hdiaq(i,k,m,a) <--
! ( -1.00000000) D3(i,m,o1,k,o2,i) V2(k,o1,m,o2)
! * Begin scaling analysis .... *
for k in {occ}:
 Read V2 from GA for k
  for a in {vir}:
   Read Hdiag from GA for a
    Hdiag_{(a)}(i, k, m) += sum(o1,o2) V2(,o1,m,o2) * D3(i,m,o1,k,o2,i)
    Accumulate Hdiag (a)(i,k,m) for a
! No.33
! Hdiaq(i,k,m,a) <--
! ( -1.00000000) D3(i,m,k,o2,m,o1) V2(i,o1,k,o2)
! * Begin scaling analysis .... *
for i in {occ}:
 Read V2 from GA for i
  for a in {vir}:
   Read Hdiag from GA for a
   Hdiag_{(a)}(i, k, m) += sum(o1,o2) V2(,o1,k,o2) * D3(i,m,k,o2,m,o1)
   Accumulate Hdiag_(a)(i,k,m) for a
! No.34
! Hdiag(i,k,m,a) <--
! (-1.00000000) D2(i,o2,k,o1) V2(i,o2,k,o1)
! * Begin scaling analysis .... *
for i in {occ}:
 Read V2 from GA for i
  for a in {vir}:
   Read Hdiag from GA for a
   Hdiag_{(a)}(i, k, m) += sum(o2,o1) V2(,o2,k,o1) * D2(i,o2,k,o1)
   Accumulate Hdiag_(a)(i,k,m) for a
! No.35
! Hdiag(i,k,m,a) <--
! ( 1.00000000) D4(i,m,k,k,m,i,o1,o2) V2(o1,o2,a,a)
! Indices of ERI are rotated to match with LHS.
```

```
eclipse sort.dat
 9 11, 12 16:46
                                                                  Page 27/145
! * Begin scaling analysis .... *
for a in {vir}:
 Read Hdiag from GA for a
 Read V2 from GA for a
 for i in {occ}:
   for m in {occ}:
     Read D4 from GA for i, m
     Hdiag_(a)(i, k, m) += sum(o1,o2) V2(,a,o1,o2) * D4(,,k,k,m,i,o1,o2)
 Accumulate Hdiag (a)(i,k,m) for a
! No.36
! Hdiaq(i,k,m,a) <--
! ( 1.00000000) D3(i,i,k,k,o1,o2) V2(o1,o2,a,a)
! Indices of ERI are rotated to match with LHS.
! * Begin scaling analysis .... *
for a in {vir}:
 Read Hdiag from GA for a
 Read V2 from GA for a
 Hdiag_(a)(i, k, m) += sum(o1,o2) V2(,a,o1,o2) * D3(i,i,k,k,o1,o2)
 Accumulate Hdiag_(a)(i,k,m) for a
! No.37
! Hdiaq(i,k,m,a) <--
! ( 2.00000000) D3(i,m,k,k,o1,i) V2(m,o1,a,a)
! Indices of ERI are rotated to match with LHS.
! * Begin scaling analysis .... *
for a in {vir}:
 Read Hdiag from GA for a
 Read V2 from GA for a
 Hdiag_(a)(i, k, m) += 2 sum(o1) V2(,a,m,o1) * D3(i,m,k,k,o1,i)
 Accumulate Hdiag (a)(i,k,m) for a
1 No. 38
! Hdiaq(i,k,m,a) <--
! ( 1.00000000) D2(i,i,k,k) V2(m,m,a,a)
! Indices of ERI are rotated to match with LHS.
! * Begin scaling analysis .... *
for a in {vir}:
 Read Hdiag from GA for a
 Read V2 from GA for a
 Hdiag_(a)(i, k, m) += sum() V2(,a,m,m) * D2(i,i,k,k)
 Accumulate Hdiag_(a)(i,k,m) for a
! No.39
! Hdiag(i,k,m,a) <--
! ( 1.00000000) D4(i,m,k,o1,m,i,o2,k) V2(o1,a,o2,a)
! Indices of ERI are rotated to match with LHS.
! * Begin scaling analysis .... *
for a in {vir}:
Read Hdiag from GA for a
 Read V2 from GA for a
 for i in {occ}:
```

```
eclipse sort.dat
  9 11, 12 16:46
                                                                   Page 28/145
    for m in {occ}:
      Read D4 from GA for i, m
      Hdiag_(a)(i, k, m) += sum(o1,o2) V2(,o1,o2,a) * D4(,,k,o1,m,i,o2,k)
  Accumulate Hdiag (a)(i,k,m) for a
! No.40
! Hdiaq(i,k,m,a) <--
! ( 1.00000000) D3(i,i,k,o1,o2,k) V2(o1,a,o2,a)
! Indices of ERI are rotated to match with LHS.
! * Begin scaling analysis .... *
for a in {vir}:
 Read Hdiag from GA for a
  Read V2 from GA for a
  Hdiag_{(a)}(i, k, m) += sum(o1,o2) V2(,o1,o2,a) * D3(i,i,k,o1,o2,k)
  Accumulate Hdiag (a)(i,k,m) for a
! No.41
! Hdiag(i,k,m,a) <--
! ( 2.00000000) D3(i,k,k,o1,m,i) V2(m,a,o1,a)
! Indices of ERI are rotated to match with LHS.
! * Begin scaling analysis .... *
for a in {vir}:
 Read Hdiag from GA for a
  Read V2 from GA for a
  Hdiag_(a)(i, k, m) += 2 sum(o1) V2(,m,o1,a) * D3(i,k,k,o1,m,i)
  Accumulate Hdiag (a)(i,k,m) for a
! No.42
! Hdiag(i,k,m,a) <--
! ( 1.00000000) D2(i,k,k,i) V2(m,a,m,a)
! Indices of ERI are rotated to match with LHS.
! * Begin scaling analysis .... *
for a in {vir}:
 Read Hdiag from GA for a
  Read V2 from GA for a
 Hdiag_{(a)}(i, k, m) += sum() V2(,m,m,a) * D2(i,k,k,i)
 Accumulate Hdiag_(a)(i,k,m) for a
! No.43
! Hdiag(i,k,m,a) <--
! ( 1.00000000) Ecas D3(i,m,k,k,m,i)
! * Begin scaling analysis .... *
for a in {vir}:
 Read Hdiag from GA for a
 Hdiag_{(a)}(i, k, m) += Ecas sum() D3(i, m, k, k, m, i)
 Accumulate Hdiag_(a)(i,k,m) for a
! No.44
! Hdiag(i,k,m,a) <--
! ( 1.00000000) Ecas D2(i,i,k,k)
```

```
eclipse sort.dat
 9 11, 12 16:46
                                                                 Page 29/145
! * Begin scaling analysis .... *
for a in {vir}:
 Read Hdiag from GA for a
 Hdiag_(a)(i, k, m) += Ecas sum() D2(i,i,k,k)
 Accumulate Hdiag (a)(i,k,m) for a
< Calculation of the Sigma {0} += <Psi0 | H T2 ER | Psi0 > >
* 1 <g/oovv>
    0.50000000) T2(o1,o2,v1,v2) V2(o3,o4,v1,v2) E2(o3,o4,o1,o2)
    0.50000000) T2(o1,o2,v1,v2) V2(o3,o4,v2,v1) E2(o3,o4,o2,o1)
Decompose RDMs .....
< RESULT >
   0: (1.00000000) D2(01,02,03,04) T2(01,02,v1,v2) V2(03,04,v1,v2)
< RESULT2 >
   0 : (1.00000000) D2(01,03,02,04) T2(01,02,v1,v2) V2(03,v1,04,v2)
   0: (1.00000000) D2(o1,o3,o2,o4) T2(o1,o2,v1,v2) V2(o3,v1,o4,v2)
Setting up parameters as default ....
8 888888888 8 8888888888
                                              ,8.
                                                       8888888 888888888 ,088
88880.
8 8888
               8 8888
                                     ,888.
                                            ,888.
                                                             8 8888
                                                                      . 8888
    `88.
 8 8888
               8 8888
                                    . `8888. . `8888.
                                                             8 8888
                                                                      ,8 8888
 8 8888
               8 8888
                                    ,8.'8888. ,8.'8888.
                                                             8 8888
                                                                      88 888
       18b
 8 88888888888 8 8888888888888
                                  ,8'8.'8888,8^8.'8888.
                                                             8 8888
                                                                      88 888
       88
                                  ,8' '8.'8888' '8.'8888.
8 8888
               8 8888
                                                             8 8888
                                                                      88 8888
 8 8888
               8 8888
                                       188.
                                                `8.`8888.
                                                             8 8888
                                                                      88 888
      ,8P
 8 8888
               8 8888
                                .8'
                                        18.17
                                                 18.18888.
                                                             8 8888
                                                                      18 8888
 8 8888
               8 8888
                               .8'
                                         ۱8
                                                  18.18888. 8 8888
                                                                       ' 8888
   ,88′
8 8888
               8 8888888888 ,8'
                                                 18.18888. 8 8888
                                                                          1888
8888P'
! * 0 terms are replaced in the linking process ....
! No.0
! SO() <--
! (1.00000000) D2(01,03,02,04) T2(01,02,v1,v2) V2(03,v1,04,v2)
! Indices of ERI are rotated to match with Bareamp.
! *** D2(01,03,02,04) T2(01,02,v1,v2) is skipped due to the priority
Case 1 .... X(o1,o2,v2,v1) <---- ( 1.00000000) D2(o1,o3,o2,o4) V2(v2,o4,o
! Polynomial order is O(o^4v^2)
! Maximum memory usage is O(o^2v^1)
Case 2 .... X(01,02,04,03) <---- ( 1.00000000) T2(01,02,v1,v2) V2(v2,04,0
3.v1)
! Polynomial order is O(o^4v^2)
! Maximum memory usage is O(o^4)
```

```
eclipse sort.dat
  9 11, 12 16:46
                                                                   Page 30/145
 ! The optimal choice is .....
1: X(o1,o2,v2,v1) <-- ( 1.00000000) D2(o1,o3,o2,o4) V2(v2,o4,o3,v1)
2: SO() < -- ( 1.00000000) T2(01,02,v1,v2) X(01,02,v2,v1)
 ! Scaling
              : O(o^4v^2)
! Max size of X : o^2v^1
 ! * Begin scaling analysis .... *
for v2 in {vir}:
  Read V2 from GA for v2
  Read T2 from GA for v2
  Declare X as a o^2v^1 tensor
  X(v_2)(0_1,0_2,v_1) += 1.0 sum(0_4,0_3) V2(,0_4,0_3,v_1) * D2(0_1,0_3,0_2,0_4)
  SO() += 1.0 sum(01,02,v1) T2(01,02,v1,) * X (v2)(01,02,v1)
 * 2 <q/ooov>
     0.50000000) T2(o1,o2,o3,v1) V2(c1,o4,c2,v1) E3(c1,o3,o4,c2,o1,o2)
     0.50000000) T2(o1,o2,o3,v1) V2(c1,c2,v1,o4) E3(c1,o3,o4,o2,o1,c2)
     0.50000000) T2(o1,o2,o3,v1) V2(c1,c2,v1,o4) E3(c1,o3,o4,o2,o1,c2)
     0.50000000) T2(o1,o2,o3,v1) V2(c1,o4,c2,v1) E3(c1,o3,o4,c2,o1,o2)
     0.50000000) T2(o1,o2,o3,v1) V2(o4,o5,o6,v1) E3(o3,o4,o5,o1,o6,o2)
     0.50000000) T2(o1,o2,o3,v1) V2(o3,o5,o4,v1) E2(o4,o5,o1,o2)
     0.50000000) T2(o1,o2,o3,v1) V2(o4,o5,v1,o6) E3(o3,o4,o5,o1,o2,o6)
     0.50000000) T2(o1,o2,o3,v1) V2(o3,o4,o5,v1) E2(o4,o5,o2,o1)
Decompose RDMs .....
 < RESULT >
    0 : (
             1.00000000) D2(o1,o2,o3,o4) T2(o2,o1,o4,v1) h(o3,v1)
    1: (
             2.00000000) D2(o4,o3,o2,o1) T2(o3,o4,o1,v1) V2(c1,o2,c1,v1)
    2 : (-1.00000000) D2(04,03,02,01) T2(04,03,02,v1) V2(c1,c1,01,v1)
    3 : (
             1.00000000) D3(01,02,03,04,05,06) T2(01,02,04,v1) V2(03,05,06,v1)
    4 : (
             1.00000000) D2(01.02.03.04) T2(01.02.05.v1) V2(03.04.05.v1)
< RESULT2 >
    0: (1.00000000) D2(o1,o3,o2,o4) T2(o2,o1,o4,v1) h(o3,v1)
             2.00000000) D2(o1,o3,o2,o4) T2(o3,o4,o1,v1) V2(c1,c1,o2,v1)
    1: (
    2: (
            -1.00000000) D2(o1,o3,o2,o4) T2(o4,o3,o2,v1) V2(c1,o1,c1,v1)
             1.00000000) D3(o1,o4,o2,o5,o3,o6) T2(o1,o2,o4,v1) V2(o3,o6,o5,v1)
    3 : (
    4: (
             1.00000000) D2(o1,o3,o2,o4) T2(o1,o2,o5,v1) V2(o3,o5,o4,v1)
< RESULT >
    0: (
             1.00000000) D2(o1,o3,o2,o4) T2(o2,o1,o4,v1) h(o3,v1)
             2.00000000) D2(o1,o3,o2,o4) T2(o3,o4,o1,v1) V2(c1,c1,o2,v1)
    2: (
            -1.00000000) D2(o1,o3,o2,o4) T2(o4,o3,o2,v1) V2(c1,o1,c1,v1)
    3 : (
            1.00000000) D3(o1,o4,o2,o5,o3,o6) T2(o1,o2,o4,v1) V2(o3,o6,o5,v1)
    4: (1.00000000) D2(o1,o3,o2,o4) T2(o1,o2,o5,v1) V2(o3,o5,o4,v1)
Setting up parameters as default ....
                                                        888888 88888888 ,088
 8 888888888 8 8888888888
                                      ,8. ,8.
88880.
                                      ,888.
 8 8888
                8 8888
                                                ,888.
                                                              8 8888
                                                                        . 8888
    `88.
 8 8888
                8 8888
                                     . `8888. . `8888.
                                                              8 8888
                                                                       ,8 8888
      18h
 8 8888
                8 8888
                                     .8.1888. .8.18888.
                                                              8 8888
                                                                       88 888
       '8b
                                                                       88 8888
 8 88888888888 8 888888888888
                                   ,8'8.'8888,8^8.'8888.
                                                              8 8888
       88
 8 8888
                8 8888
                                   ,8' '8.'8888' '8.'8888.
                                                              8 8888
                                                                       88 888
```

9 11, 12 16:46		eclipse	e_sort.da	nt	Pa	ge 31/145
8 8888	8 8888			`8.`8888.	8 8888	88 8888
,8P 8 8888	8 8888	,8′	`8.`′	`8.`8888.	8 8888	'8 8888
	8 8888	,8′	١8	`8.`8888.	8 8888	, 8888
,88' 8 8888 8888P'	8 8888888888	,8′	•	`8.`8888.	8 8888	1888
! * 2 terms are	replaced in the	e linking	process .			
1 : (2.00000 2 : (-1.00000 3 : (1.00000	nlas 1000) D2(01,03,0 1000) D2(01,03,0 1000) D2(01,03,0 1000) D3(01,04,0 1000) D2(01,03,0	02,04) T2 02,04) T2 02,05,03,	(03,04,01, (04,03,02, 06) T2(01,	v1) Y0(o2,v1) v1) Y1(o1,v1) o2,o4,v1) V2(03,06,05	,v1)
The content of e Y0 < (1.00 Y1 < (1.00	0000000) V2(c1,	c1,o2,v1)			
! No.0 ! SO() < ! (1.0000000 Case 0 X(c ! Polynomial ord ! Maximum memory Case 1 X(c ! Polynomial ord ! Maximum memory Case 2 X(c ! Polynomial ord ! Maximum memory	03,v1) < (ler is O(o^4v^1) v usage is O(o^1 o1,o2,o4,v1) <- ler is O(o^4v^1) v usage is O(o^3 02,o1,o4,o3) <- ler is O(o^4v^1)	1.00	1.000000	2(o1,o3,o2,o4 00) D2(o1,o3	,02,04)]	n(o3,v1)
! The optimal ch 1: X(o3,v1) < 2: SO() < (- (1.000000			4) T2(o2,o1,o	4,v1)	
! Scaling ! Max size of X						
! * Begin scalin	ng analysis	. *				
<pre>for v1 in {vir}: Read T2 from G Declare X as a X_(v1)(o3) +=</pre>	A for v1	o4) D2(o1	,03,02,04)	* T2(o2,o1,o	4,)	
S0_() += 1.0 s	sum(o3) X_(v1)(o	o3,) * h(o3,v1)			
!						
! No.1 ! SO() < ! (2.0000000 Case 0 X(c ! Polynomial ord ! Maximum memory Case 1 X(c ! Polynomial ord ! Maximum memory Case 2 X(c ! Polynomial ord ! Maximum memory	der is O(o^4v^1) r usage is O(o^1 r usage is O(o^1 r usage is O(o^2 der is O(o^4v^1) r usage is O(o^3 r usage is O(o^3 r usage is O(o^4v^1)	1.00		2(o1,o3,o2,o4 00) D2(o1,o3	,02,04)	04,01,v1) Y0(02,v1) Y0(02,v1)

```
eclipse sort.dat
  9 11, 12 16:46
                                                                   Page 32/145
! The optimal choice is .....
1: X(o2,v1) <-- ( 1.00000000) D2(o1,o3,o2,o4) T2(o3,o4,o1,v1)
2: SO() < -- ( 2.00000000) X(o2,v1) YO(o2,v1)
! Scaling
              : O(o^4v^1)
! Max size of X : o^1
! * Begin scaling analysis .... *
Declare Y0 as a tensor
for c1 in {core}:
 Read V2 from GA for c1
for v1 in {vir}:
  Read T2 from GA for v1
  Declare X as a o^1 tensor
 X_{(v1)(o2)} += 1.0 \text{ sum}(o1,o3,o4) D2(o1,o3,o2,o4) * T2(o3,o4,o1,)
  SO_{()} += 2 sum(o2) X_{(v1)}(o2,) * YO(o2,v1)
! No.2
! SO() <--
! ( -1.00000000) D2(o1,o3,o2,o4) T2(o4,o3,o2,v1) Y1(o1,v1)
Case 0 ..... X(o1,v1) <---- ( 1.00000000) D2(o1,o3,o2,o4) T2(o4,o3,o2,v1)
! Polynomial order is O(o^4v^1)
! Maximum memory usage is O(o^1)
Case 1 ..... X(03,02,04,v1) <---- ( 1.00000000) D2(01,03,02,04) Y1(01,v1)
! Polynomial order is O(o^4v^1)
! Maximum memory usage is O(o^3)
Case 2 ..... X(04,03,02,01) <---- ( 1.00000000) T2(04,03,02,v1) Y1(01,v1)
! Polynomial order is O(o^4v^1)
! Maximum memory usage is O(o^4)
! The optimal choice is .....
1: X(01,v1) < -- ( 1.00000000) D2(01,03,02,04) T2(04,03,02,v1)
2: SO() <-- ( -1.00000000) X(o1,v1) Y1(o1,v1)
! Scaling
              : O(o^4v^1)
! Max size of X : o^1
! * Begin scaling analysis .... *
Declare Y1 as a tensor
for c1 in {core}:
 Read V2 from GA for cl
for v1 in {vir}:
 Read T2 from GA for v1
  Declare X as a o^1 tensor
 X_{(v1)(o1)} += 1.0 \text{ sum}(o3,o2,o4) D2(o1,o3,o2,o4) * T2(o4,o3,o2,)
  SO_{()} += -1 sum(o1) X_{(v1)}(o1,) * Y1(o1,v1)
! No.3
! SO() <--
! ( 1.00000000) D3(o1,o4,o2,o5,o3,o6) T2(o1,o2,o4,v1) V2(o3,o6,o5,v1)
! Indices of ERI are rotated to match with Bareamp.
! *** D3(01,04,02,05,03,06) T2(01,02,04,v1) is skipped due to the priority
Case 1 ..... X(01,04,02,v1) < ---- ( 1.00000000) D3(01,04,02,05,03,06) V2(v)
1,05,03,06)
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^3)
```

```
eclipse sort.dat
 9 11, 12 16:46
                                                                    Page 33/145
Case 2 ..... X(o1,o2,o4,o5,o3,o6) < ---- (
                                               1.00000000) T2(o1,o2,o4,v1) V2(v
1,05,03,06)
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^6)
! The optimal choice is ..... l: X(o1,o4,o2,v1) <-- ( 1.00000000) D3(o1,o4,o2,o5,o3,o6) V2(v1,o5,o3,o6)
2: SO() <-- ( 1.00000000) T2(o1,o2,o4,v1) X(o1,o4,o2,v1)
            : O(o^6v^1)
! Scaling
! Max size of X : o^3
! * Begin scaling analysis .... *
for v1 in {vir}:
 Read V2 from GA for v1
 Read T2 from GA for v1
 Declare X as a o^3 tensor
 X_{(v1)(01,04,02)} += 1.0 \text{ sum}(05,03,06) V2(,05,03,06) * D3(01,04,02,05,03,06)
 SO() += 1.0 sum(01,02,04) T2(01,02,04) * X (v1)(01,04,02)
! No.4
! SO() <--
! (1.00000000) D2(01,03,02,04) T2(01,02,05,v1) V2(03,05,04,v1)
! Indices of ERI are rotated to match with Bareamp.
! *** D2(01,03,02,04) T2(01,02,05,v1) is skipped due to the priority
Case 1 ..... X(01,02,05,v1) <---- ( 1.00000000) D2(01,03,02,04) V2(v1,04,0)
! Polynomial order is O(o^5v^1)
! Maximum memory usage is O(o^3)
Case 2 ..... X(01,02,04,03) <---- ( 1.00000000) T2(01,02,05,v1) V2(v1,04,0
! Polynomial order is O(o^5v^1)
! Maximum memory usage is O(o^4)
! The optimal choice is .....
1: X(o1,o2,o5,v1) <-- ( 1.00000000) D2(o1,o3,o2,o4) V2(v1,o4,o3,o5)
2: S0() <-- ( 1.00000000) T2(o1,o2,o5,v1) X(o1,o2,o5,v1)
! Scaling
             : O(o^5v^1)
! Max size of X : o^3
! * Begin scaling analysis .... *
for v1 in {vir}:
 Read V2 from GA for v1
 Read T2 from GA for v1
 Declare X as a o^3 tensor
 X_{(v1)}(01,02,05) += 1.0 sum(04,03) V2(,04,03,05) * D2(01,03,02,04)
 S0_{()} += 1.0 \text{ sum}(01,02,05) T2(01,02,05,) * X_{(v1)}(01,02,05,)
< Calculation of the Sigma_{aa'}^{ee'} += <Psi0|EL H T0 |Psi0> >
* 1 <oovv/g>
     0.50000000) T0 V2(o1.o2.a.c) E2(i.k.o1.o2)
     0.50000000) T0 V2(o1,o2,c,a) E2(i,k,o2,o1)
Decompose RDMs .....
```

```
eclipse sort.dat
                                                                 Page 34/145
 9 11, 12 16:46
< RESULT >
            1.00000000) T0 D2(i,k,o1,o2) V2(o1,o2,a,c)
   0: (
< RESULT2 >
   0: (
            1.00000000) T0 D2(i,o1,k,o2) V2(o1,a,o2,c)
< RESULT >
   0 : (1.00000000) T0 D2(i,o1,k,o2) V2(o1,a,o2,c)
Setting up parameters as default ....
8 888888888 8 8888888888
                                     ,8.
                                              ,8.
                                                       8888888 888888888 ,088
88880.
8 8888
               8 8888
                                     ,888.
                                               ,888.
                                                             8 8888
                                                                      . 8888
    ۱88.
8 8888
               8 8888
                                    . '8888. . '8888.
                                                             8 8888
                                                                     ,8 8888
     '8b
8 8888
               8 8888
                                   ,8.'8888. ,8.'8888.
                                                             8 8888
                                                                     88 8888
8 88888888888 8 888888888888
                                                                     88 888
                                  ,8'8.\8888,8^8.\8888.
                                                             8 8888
       88
8 8888
               8 8888
                                 ,8' '8.'8888' '8.'8888.
                                                             8 8888
                                                                     88 888
8 8888
               8 8888
                                ,8' '8.'88'
                                               18.18888.
                                                            8 8888
                                                                     88 888
8 8888
               8 8888
                                ,8′
                                       `8.`′
                                                 `8.`8888.
                                                            8 8888
                                                                      '8 8888
     ,8P
8 8888
               8 8888
                               ,8′
                                        ۱8
                                                 18.18888. 8 8888
                                                                      '8888
   ,88′
8 8888
               8 8888888888 ,8'
                                                 18.18888. 8 8888
                                                                         1888
8888P′
! * 0 terms are replaced in the linking process ....
! No.0
! S2(i,k,a,c) <--
! ( 1.00000000) TO D2(i,o1,k,o2) V2(o1,a,o2,c)
! Indices of ERI are rotated to match with LHS.
Case 0 .... S2(i,k,c,a) <---- ( 1.00000000) D2(i,o1,k,o2) V2(c,o2,o1,a)
! Polynomial order is O(o^4v^2)
! Maximum memory usage is O(o^2v^1)
! The optimal choice is .....
1: S2(i,k,c,a) < -- (1.00000000) TO D2(i,o1,k,o2) V2(c,o2,o1,a)
! Scaling
            : O(o^4v^2)
! Max size of X : o^2v^1
! * Begin scaling analysis .... *
for c in {vir}:
 Read V2 from GA for c
 Read S2 from GA for c
 Declare S2 as a o^2v^1 tensor
 S2_{(c)}(i, k, a) += T0 sum(o2,o1) V2(,o2,o1,a) * D2(i,o1,k,o2)
 Accumulate S2_(c)(i,k,a) for c
* 2 <000v/g>
    0.50000000) T0 V2(c1,o1,c2,a) E3(c1,i,k,c2,m,o1)
    0.50000000) T0 V2(c1,c2,o1,a) E3(c1,i,k,o1,m,c2)
    0.50000000) T0 V2(o1,o3,o2,a) E3(i,k,o1,m,o3,o2)
    0.50000000) T0 V2(m,o2,o1,a) E2(i,k,o1,o2)
    0.50000000) T0 V2(c1,c2,o1,a) E3(c1,i,k,o1,m,c2)
    0.50000000) T0 V2(c1,o1,c2,a) E3(c1,i,k,c2,m,o1)
```

```
eclipse sort.dat
 9 11, 12 16:46
                                                                       Page 35/145
     0.50000000) T0 V2(o1,o2,o3,a) E3(i,k,o1,m,o2,o3)
     0.50000000) T0 V2(m,o1,o2,a) E2(i,k,o2,o1)
Decompose RDMs ....
< RESULT >
   0:(
            1.00000000) T0 D2(i,k,m,o1) h(o1,a)
    1: (
           2.00000000) T0 D2(i,k,m,o1) V2(c1,o1,c1,a)
    2: (
            -1.00000000) T0 D2(i,k,m,o1) V2(c1,c1,o1,a)
   2: ( -1.00000000) TO D2(1,K,m,O1, V2(C1,C1,O1,O1,O2,O3) 3: ( 1.00000000) TO D3(i,k,O1,m,O2,O3) V2(O1,O2,O3,a) 4: ( 1.00000000) TO D2(i,k,O1,O2) V2(m,O2,O1,a)
< RESULT2 >
   2: (
            -1.00000000) T0 D2(i,m,k,o1) V2(c1,o1,c1,a)
   3 : (
            1.00000000) T0 D3(i,m,k,o2,o1,o3) V2(o1,o3,o2,a)
    4: (
             1.00000000) T0 D2(i,o1,k,o2) V2(m,o1,o2,a)
< RESULT >
             1.00000000) T0 D2(i,m,k,o1) h(o1,a)
    0 : (
    1: (
             2.00000000) T0 D2(i,m,k,o1) V2(c1,c1,o1,a)
    2 : (-1.00000000) \text{ TO } D2(i,m,k,o1) V2(c1,o1,c1,a)
   3: (1.00000000) T0 D3(i,m,k,o2,o1,o3) V2(o1,o3,o2,a)
    4 : (1.00000000) \text{ TO } D2(i,o1,k,o2) \text{ } V2(m,o1,o2,a)
Setting up parameters as default ....
! * 2 terms are replaced in the linking process ....
The linked formulas ....
0 : (1.00000000) \text{ TO } D2(i,m,k,o1) \text{ } h(o1,a)
1 : (2.00000000) T0 D2(i,m,k,o1) Y0(o1,a)
2 : (-1.00000000) \text{ TO } D2(i,m,k,o1) \text{ Y1}(o1,a)
3 : ( 1.00000000) TO D3(i,m,k,o2,o1,o3) V2(o1,o3,o2,a) 4 : ( 1.00000000) TO D2(i,o1,k,o2) V2(m,o1,o2,a)
The content of each effective tensor ....
Y0 < -- ( 1.00000000) V2(c1,c1,o1,a)
Y1 < -- ( 1.00000000) V2(c1,o1,c1,a)
! No.0
! S2(i,k,m,a) <--
! ( 1.00000000) T0 D2(i,m,k,o1) h(o1,a)
Case 0 ..... S2(i,m,k,a) < ---- ( 1.00000000) D2(i,m,k,o1) h(o1,a)
! Polynomial order is O(o^4v^1)
! Maximum memory usage is O(o^3)
! The optimal choice is .....
1: S2(i,m,k,a) < -- (1.00000000) TO D2(i,m,k,o1) h(o1,a)
! Scaling
              : O(o^4v^1)
! Max size of X : o^3
! * Begin scaling analysis .... *
for a in {vir}:
```

```
eclipse sort.dat
  9 11, 12 16:46
                                                                    Page 36/145
  Read S2 from GA for a
  Declare S2 as a o^3 tensor
  S2 (a)(i, k, m) += T0 sum(o1) D2(i, m, k, o1) * h(o1, a)
  Accumulate S2 (a)(i,k,m) for a
! No.1
! S2(i,k,m,a) <--
! ( 2.00000000) T0 D2(i,m,k,o1) Y0(o1,a)
Case 0 ..... S2(i,m,k,a) <---- ( 1.00000000) D2(i,m,k,o1) Y0(o1,a)
! Polynomial order is O(o^4v^1)
! Maximum memory usage is O(o^3)
! The optimal choice is .....
1: S2(i,m,k,a) < -- ( 2.00000000) TO D2(i,m,k,o1) YO(o1,a)
             : O(o^4v^1)
! Max size of X : o^3
! * Begin scaling analysis .... *
Declare Y0 as a tensor
for c1 in {core}:
 Read V2 from GA for c1
for a in {vir}:
   Read S2 from GA for a
  Declare S2 as a o^3 tensor
  S2 (a)(i, k, m) += 2 T0 sum(o1) D2(i, m, k, o1) * Y0(o1, a)
  Accumulate S2_(a)(i,k,m) for a
! No.2
! S2(i,k,m,a) <--
! (-1.00000000) TO D2(i,m,k,o1) Y1(o1,a)
Case 0 .... S2(i,m,k,a) <---- ( 1.00000000) D2(i,m,k,o1) Y1(o1,a)
! Polynomial order is O(o^4v^1)
! Maximum memory usage is O(o^3)
! The optimal choice is .....
1: S2(i,m,k,a) <-- ( -1.00000000) T0 D2(i,m,k,o1) Y1(o1,a)
! Scaling : O(o^4v^1)
! Max size of X : o^3
! * Begin scaling analysis .... *
Declare Y1 as a tensor
for c1 in {core}:
 Read V2 from GA for c1
for a in {vir}:
 Read S2 from GA for a
  Declare S2 as a o^3 tensor
  S2_{(a)}(i, k, m) += T0 sum(o1) D2(i, m, k, o1) * Y1(o1, a)
 Accumulate S2 (a)(i,k,m) for a
! No.3
! S2(i,k,m,a) <--
! ( 1.00000000) TO D3(i,m,k,o2,o1,o3) V2(o1,o3,o2,a)
! Indices of ERI are rotated to match with LHS.
Case 0 ..... S2(i,m,k,a) <---- ( 1.00000000) D3(i,m,k,o2,o1,o3) V2(a,o2,o1
```

```
Page 37/145
                               eclipse_sort.dat
 9 11, 12 16:46
,03)
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^3)
! The optimal choice is .....
1: S2(i,m,k,a) < -- ( 1.00000000) T0 D3(i,m,k,o2,o1,o3) V2(a,o2,o1,o3)
             : O(o^6v^1)
! Max size of X : o^3
! * Begin scaling analysis .... *
for a in {vir}:
 Read V2 from GA for a
 Read S2 from GA for a
 Declare S2 as a o^3 tensor
 S2_{(a)}(i, k, m) += T0 sum(o2,o1,o3) V2(,o2,o1,o3) * D3(i,m,k,o2,o1,o3)
 Accumulate S2 (a)(i,k,m) for a
! S2(i,k,m,a) <--
! ( 1.00000000) TO D2(i,o1,k,o2) V2(m,o1,o2,a)
! Indices of ERI are rotated to match with LHS.
Case 0 ..... S2(i,k,m,a) < ---- ( 1.00000000) D2(i,o1,k,o2) V2(a,o2,m,o1)
! Polynomial order is O(o^5v^1)
! Maximum memory usage is O(o^3)
! The optimal choice is .....
1: S2(i,k,m,a) <-- ( 1.00000000) T0 D2(i,o1,k,o2) V2(a,o2,m,o1)
! Scaling
             : O(o^5v^1)
! Max size of X : o^3
! * Begin scaling analysis .... *
for a in {vir}:
Read V2 from GA for a
 Read S2 from GA for a
 Declare S2 as a o^3 tensor
 S2_{(a)}(i, k, m) += T0 sum(o2,o1) V2(,o2,m,o1) * D2(i,o1,k,o2)
 Accumulate S2_(a)(i,k,m) for a
< Construction of Sigma_{aa'}^{ee'} += <Psi0|EL H TR ER |Psi0> >
* 1 <oovv/oovv>
     0.50000000) T2(o1,o2,a,c) V2(c1,c2,c3,c4) E4(c1,c2,i,k,c3,c4,o1,o2)
    0.50000000) T2(01,02,c,a) V2(c1,c2,c3,c4) E4(c1,c2,i,k,c3,c4,02,o1)
    0.50000000) T2(o1,o2,a,c) V2(c1,o3,c2,o4) E4(c1,i,k,o3,c2,o1,o2,o4)
    0.50000000) T2(o1,o2,c,a) V2(c1,o3,c2,o4) E4(c1,i,k,o3,c2,o2,o1,o4)
    0.50000000) T2(o1,o2,a,c) V2(c1,c2,o4,o3) E4(c1,i,k,o3,o4,o1,o2,c2)
    0.50000000) T2(o1,o2,c,a) V2(c1,c2,o4,o3) E4(c1,i,k,o3,o4,o2,o1,c2)
    0.50000000) T2(o1,o2,v1,a) V2(c1,c,c2,v1) E3(c1,i,k,c2,o2,o1)
    0.50000000) T2(o1,o2,v1,c) V2(c1,a,c2,v1) E3(c1,i,k,c2,o1,o2)
    0.50000000) T2(o1,o2,a,v1) V2(c1,c,c2,v1) E3(c1,i,k,c2,o1,o2)
    0.50000000) T2(o1,o2,c,v1) V2(c1,a,c2,v1) E3(c1,i,k,c2,o2,o1)
    0.50000000) T2(o1,o2,v1,a) V2(c1,c2,v1,c) E3(c1,i,k,o1,o2,c2)
    0.50000000) T2(o1,o2,v1,c) V2(c1,c2,v1,a) E3(c1,i,k,o1,c2,o2)
    0.50000000) T2(o1,o2,a,v1) V2(c1,c2,v1,c) E3(c1,i,k,o2,o1,c2)
    0.50000000) T2(o1,o2,c,v1) V2(c1,c2,v1,a) E3(c1,i,k,o2,c2,o1)
     0.50000000) T2(o1,o2,a,c) V2(c1,c2,o4,o3) E4(c1,i,k,o3,o4,o1,o2,c2)
     0.50000000) T2(o1,o2,c,a) V2(c1,c2,o4,o3) E4(c1,i,k,o3,o4,o2,o1,c2)
     0.50000000) T2(01,02,a,c) V2(c1,03,c2,04) E4(c1,i,k,03,c2,01,02,04)
```

```
eclipse_sort.dat
   9 11, 12 16:46
                                                                                                               Page 38/145
        0.50000000) T2(01,02,c,a) V2(c1,03,c2,04) E4(c1,i,k,03,c2,02,01,04)
        0.50000000) T2(o1,o2,a,c) V2(o3,o4,o5,o6) E4(i,k,o3,o4,o1,o2,o5,o6)
        0.50000000) T2(o1,o2,c,a) V2(o3,o4,o5,o6) E4(i,k,o3,o4,o2,o1,o5,o6)
        0.50000000) T2(o1,o2,v1,a) V2(o3,c,o4,v1) E3(i,k,o3,o2,o1,o4)
        0.50000000) T2(o1,o2,v1,c) V2(o3,a,o4,v1) E3(i,k,o3,o1,o2,o4)
        0.50000000) T2(o1,o2,a,v1) V2(o3,c,o4,v1) E3(i,k,o3,o1,o2,o4)
        0.50000000) T2(o1,o2,c,v1) V2(o3,a,o4,v1) E3(i,k,o3,o2,o1,o4)
        0.50000000) T2(o1,o2,v1,a) V2(o3,o4,v1,c) E3(i,k,o3,o2,o4,o1)
        0.50000000) T2(o1,o2,v1,c) V2(o3,o4,v1,a) E3(i,k,o3,o4,o2,o1) 0.50000000) T2(o1,o2,a,v1) V2(o3,o4,v1,c) E3(i,k,o3,o1,o4,o2)
        0.50000000) T2(o1,o2,c,v1) V2(o3,o4,v1,a) E3(i,k,o3,o4,o1,o2)
        0.50000000) T2(o1,o2,v1,a) V2(c1,c2,v1,c) E3(c1,i,k,o1,o2,c2)
        0.50000000) T2(o1,o2,v1,c) V2(c1,c2,v1,a) E3(c1,i,k,o1,c2,o2) 0.50000000) T2(o1,o2,a,v1) V2(c1,c2,v1,c) E3(c1,i,k,o2,o1,c2)
       0.50000000) T2(o1,o2,c,v1) V2(c1,c2,v1,a) E3(c1,i,k,o2,c2,o1) 0.50000000) T2(o1,o2,v1,a) V2(c1,c,c2,v1) E3(c1,i,k,c2,o2,o1)
        0.50000000) T2(o1,o2,v1,c) V2(c1,a,c2,v1) E3(c1,i,k,c2,o1,o2)
        0.50000000) T2(o1,o2,a,v1) V2(c1,c,c2,v1) E3(c1,i,k,c2,o1,o2)
        0.50000000) T2(o1,o2,c,v1) V2(c1,a,c2,v1) E3(c1,i,k,c2,o2,o1)
        0.50000000) T2(o1,o2,v1,a) V2(o3,o4,v1,c) E3(i,k,o3,o2,o4,o1)
       0.50000000) T2(o1,o2,v1,c) V2(o3,o4,v1,a) E3(i,k,o3,o4,o2,o1) 0.50000000) T2(o1,o2,a,v1) V2(o3,o4,v1,c) E3(i,k,o3,o1,o4,o2)
        0.50000000) T2(o1,o2,c,v1) V2(o3,o4,v1,a) E3(i,k,o3,o4,o1,o2)
        0.50000000) T2(o1,o2,v1,a) V2(o3,c,o4,v1) E3(i,k,o3,o2,o1,o4)
       0.50000000) T2(o1,o2,v1,c) V2(o3,a,o4,v1) E3(i,k,o3,o1,o2,o4)
0.50000000) T2(o1,o2,a,v1) V2(o3,a,o4,v1) E3(i,k,o3,o1,o2,o4)
0.50000000) T2(o1,o2,a,v1) V2(o3,a,o4,v1) E3(i,k,o3,o1,o2,o4)
0.50000000) T2(o1,o2,v1,v2) V2(o3,a,o4,v1) E3(i,k,o3,o2,o1,o4)
0.50000000) T2(o1,o2,v1,v2) V2(a,c,v1,v2) E2(i,k,o1,o2)
0.50000000) T2(o1,o2,v1,v2) V2(a,c,v2,v1) E2(i,k,o2,o1)
        0.50000000) T2(o1,o2,v1,v2) V2(a,c,v2,v1) E2(i,k,o2,o1)
        0.50000000) T2(o1,o2,v1,v2) V2(a,c,v1,v2) E2(i,k,o1,o2)
Decompose RDMs .....
< RESULT >
                     2.00000000) D2(i,k,o2,o1) T2(o2,o1,a,c) h(c1,c1)
      1: (
                     2.00000000) D2(i,k,o2,o1) T2(o1,o2,c,a) h(c1,c1)
      2 : (
                     1.00000000) D3(i,k,o4,o3,o2,o1) T2(o3,o2,a,c) h(o4,o1)
2 : ( 1.00000000) D3(i,k,o1,o2,o1) T2(o3,o2,a,c) R(o4,o1)
3 : ( 1.00000000) D3(i,k,o1,o2,o3,o4) T2(o3,o2,c,a) h(o1,o4)
4 : ( 1.00000000) D2(i,k,o2,o1) T2(o1,o2,v1,a) h(c,v1)
5 : ( 1.00000000) D2(i,k,o2,o1) T2(o2,o1,v1,c) h(a,v1)
6 : ( 1.00000000) D2(i,k,o2,o1) T2(o2,o1,a,v1) h(c,v1)
7 : ( 1.00000000) D2(i,k,o1,o2) T2(o2,o1,a,v1) h(a,v1)
8 : ( 2.0000000) D2(i,k,o2,o1) T2(o2,o1,a,c) V2(c2,c1,c2,c1)
9 : ( -1.0000000) D2(i,k,o2,o1) T2(o2,o1,a,c) V2(c2,c1,c2,c1)
10 : ( 2.0000000) D2(i,k,o2,o1) T2(o1,o2,c,a) V2(c2,c1,c2,c1)
11 : ( -1.0000000) D2(i,k,o2,o1) T2(o1,o2,c,a) V2(c2,c2,c1,c1)
12 : ( 2.00000000) D3(i,k,o2,o1) T2(o1,o2,c,a) V2(c2,c2,c1,c1)
 12: ( 2.00000000) D3(i,k,o4,o3,o2,o1) T2(o3,o2,a,c) V2(c1,o4,c1,o1)
 13: ( 2.00000000) D3(i,k,o4,o3,o2,o1) T2(o2,o3,c,a) V2(c1,o4,c1,o1)
13 : ( 2.00000000) D3(i,k,04,03,02,01) T2(02,03,c,a) V2(c1,04,c1,01)
14 : ( -1.00000000) D3(i,k,04,03,02,01) T2(03,02,a,c) V2(c1,c1,04,01)
15 : ( -1.00000000) D3(i,k,04,03,02,01) T2(02,03,c,a) V2(c1,c1,04,01)
16 : ( 2.00000000) D2(i,k,02,01) T2(01,02,V1,a) V2(c1,c,c1,V1)
17 : ( 2.00000000) D2(i,k,02,01) T2(02,01,V1,c) V2(c1,a,c1,V1)
18 : ( 2.00000000) D2(i,k,02,01) T2(02,01,a,V1) V2(c1,c,c1,V1)
19: ( 2.00000000) D2(i,k,o2,o1) T2(o1,o2,c,v1) V2(c1,c1,c1,v1)

20: ( -1.00000000) D2(i,k,o2,o1) T2(o1,o2,c,v1,a) V2(c1,c1,c,v1)

21: ( -1.00000000) D2(i,k,o2,o1) T2(o1,o2,v1,a) V2(c1,c1,c,v1)

22: ( -1.00000000) D2(i,k,o2,o1) T2(o2,o1,v1,c) V2(c1,c1,c,v1)
    23 : ( -1.00000000) D2(i,k,o2,o1) T2(o2,o1,a,v1) V2(c1,c1,c,v1)
23 : ( -1.00000000) D2(i,k,o2,o1) T2(o1,o2,c,v1) V2(c1,c1,a,v1)
    24 : (
                     0.50000000) D4(i,k,o6,o5,o4,o3,o2,o1) T2(o4,o3,a,c) V2(o6,o5,o2,o1)
    25 : (
                     0.50000000) D4(i,k,01,02,03,04,05,06) T2(04,03,c,a) V2(01,02,05,06)
                     27 : (
    28 : (
                     1.00000000) D3(i,k,o4,o3,o2,o1) T2(o3,o2,a,v1) V2(o4,c,o1,v1)
                     1.00000000) D3(i,k,o1,o2,o3,o4) T2(o3,o2,c,v1) V2(o1,a,o4,v1)
    29 : (
    30 : (
                     1.00000000) D3(i,k,04,03,02,01) T2(01,03,v1,a) V2(04,02,v1,c)
```

```
eclipse sort.dat
   9 11, 12 16:46
                            1.00000000) D3(i,k,o4,o3,o2,o1) T2(o1,o2,v1,c) V2(o4,o3,v1,a)
                           1.00000000) D3(i,k,o4,o3,o2,o1) T2(o3,o1,a,v1) V2(o4,o2,v1,c)
                           1.00000000) D3(i,k,o1,o2,o3,o4) T2(o3,o4,c,v1) V2(o1,o2,v1,a)

1.00000000) D2(i,k,o1,o2) T2(o1,o2,v1,v2) V2(a,c,v1,v2)

1.00000000) D2(i,k,o1,o2) T2(o2,o1,v1,v2) V2(a,c,v2,v1)
      34: (
      35 : (
< RESULT2 >
                           2.00000000) D2(i,o2,k,o1) T2(o2,o1,a,c) h(c1,c1) 2.00000000) D2(i,o2,k,o1) T2(o1,o2,c,a) h(c1,c1)
        0 : (
        1: (
        2: (
                           1.00000000) D3(i,o3,k,o2,o4,o1) T2(o3,o2,a,c) h(o4,o1)
        3: (
                           1.00000000) D3(i,o2,k,o3,o1,o4) T2(o3,o2,c,a) h(o1,o4)
        4: (
                           1.00000000) D2(i,o2,k,o1) T2(o1,o2,v1,a) h(c,v1)
                           1.00000000) D2(i,o2,k,o1) T2(o2,o1,v1,c) h(a,v1)
        5: (
                           1.00000000) D2(i,o2,k,o1) T2(o2,o1,a,v1) h(c,v1)

1.00000000) D2(i,o1,k,o2) T2(o2,o1,c,v1) h(a,v1)

2.00000000) D2(i,o2,k,o1) T2(o2,o1,a,c) V2(c1,c1,c2,c2)
        6: (
        7: (
        8: (
        9: (
                         -1.00000000) D2(i,o2,k,o1) T2(o2,o1,a,c) V2(c1,c2,c1,c2)
                     -1.000000000) D2(i,o2,k,o1) T2(o2,o1,a,c) V2(c1,c2,c1,c2)
2.00000000) D2(i,o2,k,o1) T2(o1,o2,c,a) V2(c1,c1,c2,c2)
-1.00000000) D2(i,o2,k,o1) T2(o1,o2,c,a) V2(c1,c2,c1,c2)
2.00000000) D3(i,o3,k,o2,o4,o1) T2(o3,o2,a,c) V2(c1,c1,o1,o4)
2.00000000) D3(i,o3,k,o2,o4,o1) T2(o2,o3,c,a) V2(c1,c1,o1,o4)
-1.00000000) D3(i,o3,k,o2,o4,o1) T2(o3,o2,a,c) V2(c1,o1,c1,o4)
-1.00000000) D3(i,o3,k,o2,o4,o1) T2(o2,o3,c,a) V2(c1,o1,c1,o4)
-2.00000000) D3(i,o3,k,o2,o4,o1) T2(o2,o3,c,a) V2(c1,o1,c1,o4)
      11: (
      12: (
      13: (
      14: (
      15 : (
                        -1.00000000) D3(i,o3,k,o2,o4,o1) T2(o2,o3,c,a) V2(c1,o1,c2,00000000) D2(i,o2,k,o1) T2(o1,o2,v1,a) V2(c1,c1,c,v1) 2.00000000) D2(i,o2,k,o1) T2(o2,o1,v1,c) V2(c1,c1,a,v1) 2.00000000) D2(i,o2,k,o1) T2(o2,o1,a,v1) V2(c1,c1,c,v1) 2.00000000) D2(i,o2,k,o1) T2(o1,o2,c,v1) V2(c1,c1,a,v1) -1.00000000) D2(i,o2,k,o1) T2(o1,o2,v1,a) V2(c1,c,c1,v1) -1.00000000) D2(i,o2,k,o1) T2(o2,o1,v1,c) V2(c1,a,c1,v1) -1.00000000) D2(i,o2,k,o1) T2(o2,o1,v1,c) V2(c1,a,c1,v1) D2(c1,o2,v1,o1,o2,v1,o1,o2,v1,o1,o2,v1,o2,o1,o2,v1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o1,o2,o
      17: (
      18 : (
      19: (
      20 : (
      21 : (
                         -1.00000000) D2(i,o2,k,o1) T2(o2,o1,a,v1) V2(c1,c,c1,v1) -1.00000000) D2(i,o2,k,o1) T2(o1,o2,c,v1) V2(c1,a,c1,v1)
      23 : (
      24 : (
                          0.50000000) D4(i,o4,k,o3,o5,o1,o6,o2) T2(o4,o3,a,c) V2(o1,o5,o2,o6)
      25 : (
                           0.50000000) D4(i,o3,k,o4,o1,o5,o2,o6) T2(o4,o3,c,a) V2(o1,o5,o2,o6)
                           1.00000000) D3(i,o3,k,o2,o4,o1) T2(o2,o3,v1,a) V2(o1,o4,c,v1)
      27 : (
                           1.00000000) D3(i,o3,k,o2,o4,o1) T2(o3,o2,v1,c) V2(o1,o4,a,v1)
      28 : (
                           1.00000000) D3(i,o3,k,o2,o4,o1) T2(o3,o2,a,v1) V2(o1,o4,c,v1)
                           1.00000000) D3(i,o2,k,o3,o1,o4) T2(o3,o2,c,v1) V2(o1,o4,a,v1) 1.00000000) D3(i,o3,k,o2,o4,o1) T2(o1,o3,v1,a) V2(o2,c,o4,v1)
      30 : (
                           1.00000000) D3(i,o3,k,o2,o4,o1) T2(o1,o2,v1,c) V2(o3,a,o4,v1)
      31 : (
                           1.00000000) D3(i,o3,k,o2,o4,o1) T2(o3,o1,a,v1) V2(o2,c,o4,v1)
                           1.00000000) D3(i,o2,k,o3,o1,o4) T2(o3,o4,c,v1) V2(o1,v1,o2,a)
                           1.00000000) D2(i,o1,k,o2) T2(o1,o2,v1,v2) V2(a,v1,c,v2)
                           1.00000000) D2(i,o1,k,o2) T2(o2,o1,v1,v2) V2(a,v2,c,v1)
< RESHLT >
        0: (
                           2.00000000) D2(i,o2,k,o1) T2(o2,o1,a,c) h(c1,c1)
                           2.00000000) D2(i,o2,k,o1) T2(o1,o2,c,a) h(c1,c1)
        1: (
                           1.00000000) D3(i,o3,k,o2,o4,o1) T2(o3,o2,a,c) h(o4,o1)
        2: (
                           1.00000000) D3(i,o2,k,o3,o1,o4) T2(o3,o2,c,a) h(o1,o4) 1.00000000) D2(i,o2,k,o1) T2(o1,o2,v1,a) h(c,v1)
        4: (
                           1.00000000) D2(i,o2,k,o1) T2(o2,o1,v1,c) h(a,v1)
        5 : (
                           1.00000000) D2(i,o2,k,o1) T2(o2,o1,a,v1) h(c,v1)
                          1.00000000) D2(i,o1,k,o2) T2(o2,o1,c,v1) h(a,v1)
        7: (
                        2.00000000) D2(i,o2,k,o1) T2(o2,o1,a,c) V2(c1,c1,c2,c2)
        8 : (
                        -1.00000000) D2(i,o2,k,o1) T2(o2,o1,a,c) V2(c1,c2,c1,c2) 2.00000000) D2(i,o2,k,o1) T2(o1,o2,c,a) V2(c1,c1,c2,c2)
        9: (
      10: (
                         -1.00000000) D2(i,o2,k,o1) T2(o1,o2,c,a) V2(c1,c2,c1,c2)
      11: (
                        2.00000000) D3(i,o3,k,o2,o4,o1) T2(o3,o2,a,c) V2(c1,c1,o1,o4) 2.00000000) D3(i,o3,k,o2,o4,o1) T2(o2,o3,c,a) V2(c1,c1,o1,o4)
                        2.000000000 D3(i,o3,k,o2,o4,o1) T2(o3,o2,a,c) V2(c1,c1,c1,o4)
-1.00000000 D3(i,o3,k,o2,o4,o1) T2(o2,o3,c,a) V2(c1,o1,c1,o4)
-1.00000000 D3(i,o3,k,o2,o4,o1) T2(o2,o3,c,a) V2(c1,o1,c1,o4)
2.00000000 D2(i,o2,k,o1) T2(o1,o2,v1,a) V2(c1,c1,c,v1)
                           2.00000000) D2(i,o2,k,o1) T2(o2,o1,v1,c) V2(c1,c1,a,v1)
      17 : (
      18: (
                           2.00000000) D2(i,o2,k,o1) T2(o2,o1,a,v1) V2(c1,c1,c,v1)
                         2.00000000) D2(i,o2,k,o1) T2(o1,o2,c,v1) V2(c1,c1,a,v1)
      20 : (-1.00000000) D2(i,o2,k,o1) T2(o1,o2,v1,a) V2(c1,c,c1,v1)
```

```
eclipse sort.dat
   9 11, 12 16:46
                                                                                                 Page 40/145
                  -1.00000000) D2(i,o2,k,o1) T2(o2,o1,v1,c) V2(c1,a,c1,v1)
                  -1.00000000) D2(i,o2,k,o1) T2(o2,o1,a,v1) V2(c1,c,c1,v1)
                  -1.00000000) D2(i,o2,k,o1) T2(o1,o2,c,v1) V2(c1,a,c1,v1)
     24: (
                   0.50000000) D4(i,o4,k,o3,o5,o1,o6,o2) T2(o4,o3,a,c) V2(o1,o5,o2,o6)
                   0.50000000) D4(i,o3,k,o4,o1,o5,o2,o6) T2(o4,o3,c,a) V2(o1,o5,o2,o6)
     26 : (
                   1.00000000) D3(i,o3,k,o2,o4,o1) T2(o2,o3,v1,a) V2(o1,o4,c,v1)
                  1.00000000) D3(i,o3,k,o2,o4,o1) T2(o3,o2,v1,c) V2(o1,o4,a,v1)

1.00000000) D3(i,o3,k,o2,o4,o1) T2(o3,o2,a,v1) V2(o1,o4,c,v1)

1.00000000) D3(i,o2,k,o3,o1,o4) T2(o3,o2,c,v1) V2(o1,o4,a,v1)
     28 : (
     29 : (
                   1.00000000) D3(i,o3,k,o2,o4,o1) T2(o1,o3,v1,a) V2(o2,c,o4,v1)
     30 : (
                   1.00000000) D3(i,o3,k,o2,o4,o1) T2(o1,o2,v1,c) V2(o3,a,o4,v1) 1.00000000) D3(i,o3,k,o2,o4,o1) T2(o3,o1,a,v1) V2(o2,c,o4,v1)
     31 : (
     32 : (
    33 : ( 1.00000000) D3(i,o2,k,o3,o1,o4) T2(o3,o4,c,v1) V2(o1,v1,o2,a) 34 : ( 1.00000000) D2(i,o1,k,o2) T2(o1,o2,v1,v2) V2(a,v1,c,v2) 35 : ( 1.00000000) D2(i,o1,k,o2) T2(o2,o1,v1,v2) V2(a,v2,c,v1)
Setting up parameters as default ....
! * 18 terms are replaced in the linking process ....
The linked formulas ....
0: ( 2.0000000) Y0 D2(i,o2,k,o1) T2(o2,o1,a,c) 
1: ( 2.00000000) Y1 D2(i,o2,k,o1) T2(o1,o2,c,a)
2: (
             1.00000000) D3(i,o3,k,o2,o4,o1) T2(o3,o2,a,c) h(o4,o1)
            1.00000000) D3(i,o2,k,o3,o1,o4) T2(o3,o2,c,a) h(o1,o4) 1.00000000) D2(i,o2,k,o1) T2(o1,o2,v1,a) h(c,v1) 1.00000000) D2(i,o2,k,o1) T2(o2,o1,v1,c) h(a,v1)
3 : (
4 : (
5 : (
6: ( 1.00000000) D2(i,o2,k,o1) T2(o2,o1,a,v1) h(c,v1) 
7: ( 1.00000000) D2(i,o1,k,o2) T2(o2,o1,c,v1) h(a,v1)
8: ( 2.00000000) Y2 D2(i,o2,k,o1) T2(o2,o1,a,c)

9: ( -1.00000000) Y3 D2(i,o2,k,o1) T2(o2,o1,a,c)

10: ( 2.00000000) Y4 D2(i,o2,k,o1) T2(o1,o2,c,a)
            -1.00000000) Y5 D2(i,o2,k,o1) T2(o1,o2,c,a)
11 : (
12: ( 2.00000000) D3(i,o3,k,o2,o4,o1) T2(o3,o2,a,c) Y6(o1,o4)
13 : ( 2.00000000) D3(i,o3,k,o2,o4,o1) T2(o2,o3,c,a) Y7(o1,o4)
            -1.00000000) D3(i,o3,k,o2,o4,o1) T2(o3,o2,a,c) Y8(o1,o4)
14: (
            -1.00000000) D3(i,o3,k,o2,o4,o1) T2(o2,o3,c,a) Y9(o1,o4)
15 : (
16: ( 2.00000000) D2(i,o2,k,o1) T2(o1,o2,v1,a) Y10(c,v1)
17: ( 2.00000000) D2(i,o2,k,o1) T2(o2,o1,v1,c) Y11(a,v1)
           2.00000000) D2(i,o2,k,o1) T2(o2,o1,a,v1) Y12(c,v1) 2.00000000) D2(i,o2,k,o1) T2(o1,o2,c,v1) Y13(a,v1)
18 : (
19 : (
20 : (
            -1.00000000) D2(i,o2,k,o1) T2(o1,o2,v1,a) Y14(c,v1)
            -1.00000000) D2(i,o2,k,o1) T2(o2,o1,v1,c) Y15(a,v1) -1.00000000) D2(i,o2,k,o1) T2(o2,o1,a,v1) Y16(c,v1)
21 : (
22 : (
            -1.00000000) D2(i,o2,k,o1) T2(o1,o2,c,v1) Y17(a,v1)
23 : (
24 : (
            0.50000000) D4(i,o4,k,o3,o5,o1,o6,o2) T2(o4,o3,a,c) V2(o1,o5,o2,o6)
            0.50000000) D4(i,o3,k,o4,o1,o5,o2,o6) T2(o4,o3,c,a) V2(o1,o5,o2,o6)
25 : (
26 : (
            1.00000000) D3(i,o3,k,o2,o4,o1) T2(o2,o3,v1,a) V2(o1,o4,c,v1)
            1.00000000) D3(i,o3,k,o2,o4,o1) T2(o3,o2,v1,c) V2(o1,o4,a,v1) 1.00000000) D3(i,o3,k,o2,o4,o1) T2(o3,o2,a,v1) V2(o1,o4,a,v1) 1.00000000) D3(i,o2,k,o3,o1,o4) T2(o3,o2,c,v1) V2(o1,o4,a,v1)
27 : (
28 : (
29 : (
            1.00000000) D3(i,o3,k,o2,o4,o1) T2(o1,o3,v1,a) V2(o2,c,o4,v1) 1.00000000) D3(i,o3,k,o2,o4,o1) T2(o1,o2,v1,c) V2(o3,a,o4,v1)
31 : (
32 : (
             1.00000000) D3(i,o3,k,o2,o4,o1) T2(o3,o1,a,v1) V2(o2,c,o4,v1)
33 : ( 1.00000000) D3(i,o2,k,o3,o1,o4) T2(o3,o4,c,v1) V2(o1,v1,o2,a) 
34 : ( 1.00000000) D2(i,o1,k,o2) T2(o1,o2,v1,v2) V2(a,v1,c,v2) 
35 : ( 1.00000000) D2(i,o1,k,o2) T2(o2,o1,v1,v2) V2(a,v2,c,v1)
The content of each effective tensor ....
Y0 < -- ( 1.00000000) h(c1,c1)
```

```
eclipse_sort.dat
 9 11, 12 16:46
                                                                      Page 41/145
Y1 <-- (
            1.00000000) h(c1,c1)
            1.00000000) V2(c1,c1,c2,c2)
Y2 <-- (
Y3 <-- (
            1.00000000) V2(c1,c2,c1,c2)
            1.00000000) V2(c1,c1,c2,c2)
Y4 <-- (
            1.00000000) V2(c1,c2,c1,c2)
Y5 <-- (
Y6 <-- (
          1.00000000) V2(c1,c1,o1,o4)
Y7 <-- (
          1.00000000) V2(c1,c1,o1,o4)
          1.00000000) V2(c1,o1,c1,o4)
Y8 <-- (
Y9 <-- (
            1.00000000) V2(c1,o1,c1,o4)
Y10 <-- ( 1.00000000) V2(c1,c1,c,v1)
Y11 <-- ( 1.00000000) V2(c1,c1,c,v1)
Y12 <-- (
             1.00000000) V2(c1,c1,c,v1)
Y13 <-- (
             1.00000000) V2(c1,c1,a,v1)
             1.00000000) V2(c1,c,c1,v1)
Y14 <-- (
Y15 <-- (
            1.00000000) V2(c1,a,c1,v1)
1.00000000) V2(c1,c,c1,v1)
Y16 < -- ( 1.00000000) V2(c1,c,c1,v1)

Y17 < -- ( 1.00000000) V2(c1,a,c1,v1)
! No.0
! S2(i,k,a,c) <--
! ( 2.00000000) Y0 D2(i,o2,k,o1) T2(o2,o1,a,c)
! Indices of BareAmp are rotated to match with LHS.
Case 0 ..... S2(i,k,a,c) <---- ( 1.00000000) D2(i,o2,k,o1) T2(o2,o1,a,c)
! Polynomial order is O(o^4v^2)
! Maximum memory usage is O(o^2v^1)
! The optimal choice is .....
1: S2(i,k,a,c) <-- ( 2.00000000) Y0 D2(i,o2,k,o1) T2(o2,o1,a,c)
! Scaling
              : O(o^4v^2)
! Max size of X : o^2v^1
! * Begin scaling analysis .... *
Declare YO as a scalar
for c in {vir}:
 Read T2 from GA for c
 Read S2 from GA for c
 Declare S2 as a o^2v^1 tensor
 S2_{(c)}(i, k, a) += 2 Y0 sum(o2,o1) D2(i,o2,k,o1) * T2(o2,o1,a,)
 Accumulate S2 (c)(i,k,a) for c
! No.1
! S2(i,k,a,c) <--
! ( 2.00000000) Y1 D2(i,o2,k,o1) T2(o1,o2,c,a)
Case 0 ..... S2(i,k,c,a) < ---- ( 1.00000000) D2(i,o2,k,o1) T2(o1,o2,c,a)
! Polynomial order is O(o^4v^2)
! Maximum memory usage is O(o^2)
! The optimal choice is .....
1: S2(i,k,c,a) < -- (2.00000000) Y1 D2(i,o2,k,o1) T2(o1,o2,c,a)
! Scaling
             : O(o^4v^2)
! Max size of X : o^2
! * Begin scaling analysis .... *
Declare Y1 as a scalar
for c in {vir}:
 Read S2 from GA for c
 for a in {vir}:
   Read T2 from GA for a
    Declare S2 as a o^2 tensor
```

```
eclipse sort.dat
                                                                        Page 42/145
  9 11, 12 16:46
    S2_{(c)(i, k, a)} += 2 Y1 \frac{sum(o2,o1) D2(i,o2,k,o1) * T2(o1,o2,c,)}{sum(o2,o1) D2(i,o2,k,o1) * D2(i,o2,k,o1)}
  Accumulate S2_(c)(i,k,a) for c
! No.2
! S2(i,k,a,c) <--
! ( 1.00000000) D3(i,o3,k,o2,o4,o1) T2(o3,o2,a,c) h(o4,o1)
! Indices of BareAmp are rotated to match with LHS.
Case 0 ..... X(i,k,o4,o1,a,c) < ---- ( 1.00000000) D3(i,o3,k,o2,o4,o1) T2(o
3,o2,a,c)
! Polynomial order is O(o^6v^2)
! Maximum memory usage is O(o^4v^1)
Case 1 ..... X(i,03,k,02) < ---- ( 1.00000000) D3(i,03,k,02,04,01) h(04,01)
! Polynomial order is O(o^4v^2)
! Maximum memory usage is O(o^4)
Case 2 ..... X(03,02,04,01,a,c) < ---- ( 1.00000000) T2(03,02,a,c) h(04,01)
! Polynomial order is O(o^6v^2)
! Maximum memory usage is O(o^4v^1)
! The optimal choice is .....
1: X(i,o3,k,o2) <-- ( 1.00000000) D3(i,o3,k,o2,o4,o1) h(o4,o1)

2: S2(i,k,a,c) <-- ( 1.00000000) T2(o3,o2,a,c) X(i,o3,k,o2)
! Scaling
               : O(o^4v^2)
! Max size of X : o^4
! * Begin scaling analysis .... *
Declare X as a o^4 tensor
X()(i,o3,k,o2) += 1.0 sum(o4,o1) D3(i,o3,k,o2,o4,o1) * h(o4,o1)
for c in {vir}:
 Read S2 from GA for c
  Read T2 from GA for c
  S2_{(c)}(i,k,a) += 1.0 sum(03,02) T2(03,02,a,) * X_{(i,03,k,02)}
  Accumulate S2_(c)(i,k,a) for c
! S2(i,k,a,c) <--
! (1.00000000) D3(i,o2,k,o3,o1,o4) T2(o3,o2,c,a) h(o1,o4)
Case 0 \dots X(i,k,01,04,C,a) < ---- ( 1.00000000) D3(i,02,k,03,01,04) T2(0)
3,o2,c,a)
! Polynomial order is O(o^6v^2)
! Maximum memory usage is O(o^4)
Case 1 ..... X(i,02,k,03) < ---- (1.00000000) D3(i,02,k,03,01,04) h(01,04)
! Polynomial order is O(o^4v^2)
! Maximum memory usage is O(o^4)
Case 2 ..... X(03,02,01,04,c,a) < ---- ( 1.00000000) T2(03,02,c,a) h(01,04)
! Polynomial order is O(o^6v^2)
! Maximum memory usage is O(o^4)
Factorize: Conflict between choices of optimal memory usage and polynomial order
! The optimal choice is .....
1: X(i,o2,k,o3) <-- ( 1.00000000) D3(i,o2,k,o3,o1,o4) h(o1,o4) 
2: S2(i,k,a,c) <-- ( 1.00000000) T2(o3,o2,c,a) X(i,o2,k,o3)
! Scaling
                : O(o^4v^2)
```

```
eclipse_sort.dat
 9 11, 12 16:46
                                                                    Page 43/145
! Max size of X : o^4
! * Begin scaling analysis .... *
Declare X as a o^4 tensor
X_{(i,02,k,03)} += 1.0 \text{ sum}(01,04) D3(i,02,k,03,01,04) * h(01,04)
for c in {vir}:
 Read S2 from GA for c
 for a in {vir}
   Read T2 from GA for a
   S2_{(c)(i,k,a)} += 1.0 sum(o3,o2) T2(o3,o2,c,) * X_{(i,o2,k,o3)}
   Accumulate S2 (c)(i,k,a) for c
! No.4
! S2(i,k,a,c) <--
! ( 1.00000000) D2(i,o2,k,o1) T2(o1,o2,v1,a) h(c,v1)
Case 0 ..... X(i,k,v1,a) < ---- (1.00000000) D2(i,o2,k,o1) T2(o1,o2,v1,a)
! Polynomial order is O(o^4v^2)
! Maximum memory usage is O(o^2v^1)
Case 1 ..... X(i,o2,k,o1,c,v1) <---- ( 1.00000000) D2(i,o2,k,o1) h(c,v1)
! Polynomial order is O(o^4v^3)
! Maximum memory usage is O(o^4v^1)
Case 2 ..... X(o1,o2,a,c) <---- ( 1.00000000) T2(o1,o2,v1,a) h(c,v1)
! Polynomial order is O(o^4v^2)
! Maximum memory usage is O(o^2)
Factorize: Conflict between choices of optimal memory usage and polynomial order
! The optimal choice is .....
1: X(i,k,v1,a) <-- ( 1.00000000) D2(i,o2,k,o1) T2(o1,o2,v1,a)

2: S2(i,k,a,c) <-- ( 1.00000000) X(i,k,v1,a) h(c,v1)
! Scaling
              : O(o^4v^2)
! Max size of X : o^2v^1
! * Begin scaling analysis .... *
for a in {vir}:
 Read T2 from GA for a
 Declare X as a o^2v^1 tensor
 X (a)(i,k,v1) += 1.0 sum(o2.o1) D2(i,o2,k,o1) * T2(o1,o2,v1,)
 for c in {vir}:
   Read S2 from GA for c
   S2_{(c)}(i,k,a) += 1.0 sum(v1) X_{(a)}(i,k,v1,) * h(c,v1)
   Accumulate S2_(c)(i,k,a) for c
! No.5
! S2(i,k,a,c) <--
! ( 1.00000000) D2(i,o2,k,o1) T2(o2,o1,v1,c) h(a,v1)
! Indices of BareAmp are rotated to match with LHS.
Case 0 ..... X(i,k,v1,c) <---- ( 1.00000000) D2(i,o2,k,o1) T2(o2,o1,v1,c)
! Polynomial order is O(o^4v^2)
! Maximum memory usage is O(o^2v^1)
Case 1 ..... X(i,02,k,01,a,v1) < ---- ( 1.00000000) D2(i,02,k,01) h(a,v1)
! Polynomial order is O(o^4v^3)
! Maximum memory usage is O(o^4v^2)
Case 2 ..... X(o2,o1,c,a) < ---- ( 1.00000000) T2(o2,o1,v1,c) h(a,v1)
```

```
eclipse sort.dat
  9 11, 12 16:46
                                                                        Page 44/145
! Polynomial order is O(o^4v^2)
! Maximum memory usage is O(o^2v^1)
! The optimal choice is .....
1: X(i,k,v1,c) < -- ( 1.00000000) D2(i,o2,k,o1) T2(o2,o1,v1,c) 2: S2(i,k,a,c) < -- ( 1.00000000) X(i,k,v1,c) h(a,v1)
              : O(o^4v^2)
! Scaling
! Max size of X : o^2v^1
! * Begin scaling analysis .... *
for c in {vir}:
  Read T2 from GA for c
  Read S2 from GA for c
  Declare X as a o^2v^1 tensor
  X_{(c)(i,k,v1)} += 1.0 \text{ sum}(02,01) D2(i,02,k,01) * T2(02,01,v1,)
  S2_{(c)(i,k,a)} += 1.0 sum(v1) X_{(c)(i,k,v1,)} * h(a,v1)
  Accumulate S2 (c)(i,k,a) for c
! No.6
! S2(i,k,a,c) <--
! ( 1.00000000) D2(i,o2,k,o1) T2(o2,o1,a,v1) h(c,v1)
Case 0 ..... X(i,k,a,v1) <---- ( 1.00000000) D2(i,o2,k,o1) T2(o2,o1,a,v1)
! Polynomial order is O(o^4v^2)
! Maximum memory usage is O(o^2v^1)
Case 1 ..... X(i,o2,\bar{k},o1,c,v1) <---- ( 1.00000000) D2(i,o2,k,o1) h(c,v1)
! Polynomial order is O(o^4v^3)
! Maximum memory usage is O(o^4)
Case 2 ..... X(o2,o1,a,c) <---- ( 1.00000000) T2(o2,o1,a,v1) h(c,v1)
! Polynomial order is O(o^4v^2)
! Maximum memory usage is O(o^2v^1)
! The optimal choice is .....
1: X(i,k,a,v1) < -- ( 1.00000000) D2(i,o2,k,o1) T2(o2,o1,a,v1) 2: S2(i,k,a,c) < -- ( 1.00000000) X(i,k,a,v1) h(c,v1)
! Scaling
              : O(o^4v^2)
! Max size of X : o^2v^1
! * Begin scaling analysis .... *
for v1 in {vir}:
  Read T2 from GA for v1
  Declare X as a o^2v^1 tensor
  X_{(v1)}(i,k,a) += 1.0 \text{ sum}(0.02,0.1) D2(i,0.02,k,0.1) * T2(0.02,0.1,a,)
  for c in {vir}:
   Read S2 from GA for c
    S2_{(c)}(i,k,a) += 1.0 sum() X_{(v1)}(i,k,a,) * h(c,v1)
   Accumulate S2_(c)(i,k,a) for c
! No.7
! S2(i,k,a,c) <--
! ( 1.00000000) D2(i,o1,k,o2) T2(o2,o1,c,v1) h(a,v1)
Case 0 ..... X(i,k,c,v1) <---- ( 1.00000000) D2(i,o1,k,o2) T2(o2,o1,c,v1)
! Polynomial order is O(o^4v^2)
! Maximum memory usage is O(o^2)
```

```
eclipse sort.dat
 9 11, 12 16:46
                                                                    Page 45/145
Case 1 .... X(i,o1,k,o2,a,v1) <---- (
                                            1.00000000) D2(i,o1,k,o2) h(a,v1)
! Polynomial order is O(o^4v^3)
! Maximum memory usage is O(o^4v^1)
Case 2 ..... X(02,01,c,a) < ---- (1.00000000) T2(02,01,c,v1) h(a,v1)
! Polynomial order is O(o^4v^2)
! Maximum memory usage is O(o^2v^1)
! The optimal choice is .....
1: X(i,k,c,v1) < -- ( 1.00000000) D2(i,o1,k,o2) T2(o2,o1,c,v1) 2: S2(i,k,a,c) < -- ( 1.00000000) X(i,k,c,v1) h(a,v1)
! Scaling
            : O(o^4v^2)
! Max size of X : o^2
! * Begin scaling analysis .... *
for c in {vir}:
 Read S2 from GA for c
 for v1 in {vir}:
   Read T2 from GA for v1
    Declare X as a o^2 tensor
   X(c,v1)(i,k) += 1.0 sum(o1,o2) D2(i,o1,k,o2) * T2(o2,o1,c,)
    S2_{c}(c)(i,k,a) += 1.0 sum() X_{c}(c,v1)(i,k,,) * h(a,v1)
    Accumulate S2 (c)(i,k,a) for c
! No.8
! S2(i,k,a,c) <--
! ( 2.00000000) Y2 D2(i,o2,k,o1) T2(o2,o1,a,c)
! Indices of BareAmp are rotated to match with LHS.
Case 0 ..... S2(i,k,a,c) < ---- ( 1.00000000) D2(i,o2,k,o1) T2(o2,o1,a,c)
! Polynomial order is O(o^4v^2)
! Maximum memory usage is O(o^2v^1)
! The optimal choice is .....
1: S2(i,k,a,c) <-- ( 2.00000000) Y2 D2(i,o2,k,o1) T2(o2,o1,a,c)
! Scaling
              : O(o^4v^2)
! Max size of X : o^2v^1
! * Begin scaling analysis .... *
Declare Y2 as a scalar
for c1 in {core}:
 Read V2 from GA for c1
for c in {vir}:
 Read T2 from GA for c
 Read S2 from GA for c
 Declare S2 as a o^2v^1 tensor
 S2_{(c)}(i, k, a) += 2 Y2 sum(o2,o1) D2(i,o2,k,o1) * T2(o2,o1,a,)
 Accumulate S2_(c)(i,k,a) for c
! S2(i,k,a,c) <--
! ( -1.00000000) Y3 D2(i,o2,k,o1) T2(o2,o1,a,c)
! Indices of BareAmp are rotated to match with LHS.
Case 0 ..... S2(i,k,a,c) < ---- ( 1.00000000) D2(i,o2,k,o1) T2(o2,o1,a,c)
! Polynomial order is O(o^4v^2)
! Maximum memory usage is O(o^2v^1)
```

```
eclipse sort.dat
  9 11, 12 16:46
                                                                   Page 46/145
! The optimal choice is .....
1: S2(i,k,a,c) < -- ( -1.00000000) Y3 D2(i,o2,k,o1) T2(o2,o1,a,c)
              : O(o^4v^2)
! Max size of X : o^2v^1
! * Begin scaling analysis .... *
Declare Y3 as a scalar
for c1 in {core}:
 Read V2 from GA for c1
for c in {vir}:
 Read T2 from GA for c
  Read S2 from GA for c
  Declare S2 as a o^2v^1 tensor
  S2_{(c)}(i, k, a) += Y3 sum(o2,o1) D2(i,o2,k,o1) * T2(o2,o1,a,)
 Accumulate S2 (c)(i,k,a) for c
! No.10
! S2(i,k,a,c) <--
! ( 2.00000000) Y4 D2(i,o2,k,o1) T2(o1,o2,c,a)
Case 0 ..... S2(i,k,c,a) < ---- ( 1.00000000) D2(i,o2,k,o1) T2(o1,o2,c,a)
! Polynomial order is O(o^4v^2)
! Maximum memory usage is O(o^2)
! The optimal choice is .....
1: S2(i,k,c,a) < -- (2.00000000) Y4 D2(i,o2,k,o1) T2(o1,o2,c,a)
! Scaling
             : O(o^4v^2)
! Max size of X : o^2
! * Begin scaling analysis .... *
Declare Y4 as a scalar
for c1 in {core}:
Read V2 from GA for c1
for c in {vir}:
 Read S2 from GA for c
  for a in {vir}:
   Read T2 from GA for a
   Declare S2 as a o^2 tensor
   S2 (c)(i, k, a) += 2 Y4 sum(o2,o1) D2(i,o2,k,o1) * T2(o1,o2,c,)
 Accumulate S2_(c)(i,k,a) for c
! No.11
! S2(i,k,a,c) <--
! ( -1.00000000) Y5 D2(i,o2,k,o1) T2(o1,o2,c,a)
Case 0 ..... S2(i,k,c,a) < ---- ( 1.00000000) D2(i,o2,k,o1) T2(o1,o2,c,a)
! Polynomial order is O(o^4v^2)
! Maximum memory usage is O(o^2)
! The optimal choice is .....
1: S2(i,k,c,a) < -- (-1.00000000) Y5 D2(i,o2,k,o1) T2(o1,o2,c,a)
! Scaling : O(o^4v^2)
! Max size of X : o^2
! * Begin scaling analysis .... *
Declare Y5 as a scalar
for c1 in {core}:
```

```
eclipse sort.dat
 9 11. 12 16:46
                                                                    Page 47/145
 Read V2 from GA for c1
for c in {vir}:
 Read S2 from GA for c
 for a in {vir}:
   Read T2 from GA for a
    Declare S2 as a o^2 tensor
    S2_{(c)}(i, k, a) += Y5 sum(o2,o1) D2(i,o2,k,o1) * T2(o1,o2,c,)
 Accumulate S2_(c)(i,k,a) for c
! No.12
! S2(i,k,a,c) <--
! ( 2.00000000) D3(i,o3,k,o2,o4,o1) T2(o3,o2,a,c) Y6(o1,o4)
! Indices of BareAmp are rotated to match with LHS.
Case 0 ..... X(i,k,o4,o1,a,c) <---- ( 1.00000000) D3(i,o3,k,o2,o4,o1) T2(o
! Polynomial order is O(o^6v^2)
! Maximum memory usage is O(o^4v^1)
Case 1 .... X(i, 03, k, 02) < ---- (1.00000000) D3(i, 03, k, 02, 04, 01) Y6(01, 04
! Polynomial order is O(o^4v^2)
! Maximum memory usage is O(o^4)
Case 2 ..... X(o3,o2,o1,o4,a,c) <---- ( 1.00000000) T2(o3,o2,a,c) Y6(o1,o4
! Polynomial order is O(o^6v^2)
! Maximum memory usage is O(o^4v^1)
! The optimal choice is .....
1: X(i,o3,k,o2) <-- ( 1.00000000) D3(i,o3,k,o2,o4,o1) Y6(o1,o4) 2: S2(i,k,a,c) <-- ( 2.00000000) T2(o3,o2,a,c) X(i,o3,k,o2)
! Scaling
            : O(o^4v^2)
! Max size of X : o^4
! * Begin scaling analysis .... *
Declare Y6 as a tensor
for c1 in {core}:
 Read V2 from GA for c1
Declare X as a o^4 tensor
X_{()}(i,o3,k,o2) += 1.0 sum(o4,o1) D3(i,o3,k,o2,o4,o1) * Y6(o1,o4)
for c in {vir}:
 Read S2 from GA for c
 Read T2 from GA for c
 S2_{(c)}(i,k,a) += 2 sum(03,02) T2(03,02,a,) * X_{(i)}(i,03,k,02)
 Accumulate S2_(c)(i,k,a) for c
! No.13
! S2(i,k,a,c) <--
! ( 2.00000000) D3(i,o3,k,o2,o4,o1) T2(o2,o3,c,a) Y7(o1,o4)
Case 0 ..... X(i,k,o4,o1,c,a) <---- ( 1.00000000) D3(i,o3,k,o2,o4,o1) T2(o
! Polynomial order is O(o^6v^2)
! Maximum memory usage is O(o^4)
Case 1 ..... X(i,03,k,02) < ---- (1.00000000) D3(i,03,k,02,04,01) Y7(01,04
! Polynomial order is O(o^4v^2)
! Maximum memory usage is O(o^4)
Case 2 ..... X(02,03,01,04,c,a) < ---- ( 1.00000000) T2(02,03,c,a) Y7(01,04)
```

```
eclipse sort.dat
  9 11, 12 16:46
                                                                        Page 48/145
! Polynomial order is O(o^6v^2)
! Maximum memory usage is O(o^4)
Factorize: Conflict between choices of optimal memory usage and polynomial order
! The optimal choice is .....
1: X(i,o3,k,o2) <-- ( 1.00000000) D3(i,o3,k,o2,o4,o1) Y7(o1,o4) 
2: S2(i,k,a,c) <-- ( 2.00000000) T2(o2,o3,c,a) X(i,o3,k,o2)
! Scaling
              : O(o^4v^2)
! Max size of X : o^4
! * Begin scaling analysis .... *
Declare Y7 as a tensor
for cl in {core}:
 Read V2 from GA for c1
Declare X as a o^4 tensor
X_{()}(i,o3,k,o2) += 1.0 sum(o4,o1) D3(i,o3,k,o2,o4,o1) * Y7(o1,o4)
for c in {vir}:
 Read S2 from GA for c
  for a in {vir}
    Read T2 from GA for a
    S2_{(c)(i,k,a)} += 2 sum(o2,o3) T2(o2,o3,c,) * X_{(i,o3,k,o2)}
    Accumulate S2 (c)(i,k,a) for c
! No.14
! S2(i,k,a,c) <--
[...] ( -1.00000000) D3(i,o3,k,o2,o4,o1) T2(o3,o2,a,c) Y8(o1,o4)
! Indices of BareAmp are rotated to match with LHS.
Case 0 ..... X(i,k,o4,o1,a,c) <---- ( 1.00000000) D3(i,o3,k,o2,o4,o1) T2(o
3,o2,a,c)
! Polynomial order is O(o^6v^2)
! Maximum memory usage is O(o^4v^1)
Case 1 .... X(i, 03, k, 02) < ---- (1.00000000) D3(i, 03, k, 02, 04, 01) Y8(01, 04)
! Polynomial order is O(o^4v^2)
! Maximum memory usage is O(o^4)
Case 2 .... X(03,02,01,04,a,c) <---- ( 1.00000000) T2(03,02,a,c) Y8(01,04
! Polynomial order is O(o^6v^2)
! Maximum memory usage is O(o^4v^1)
! The optimal choice is .....
1: X(i,o3,k,o2) <-- ( 1.00000000) D3(i,o3,k,o2,o4,o1) Y8(o1,o4) 
2: S2(i,k,a,c) <-- ( -1.00000000) T2(o3,o2,a,c) X(i,o3,k,o2)
! Scaling
               : O(o^4v^2)
! Max size of X : o^4
! * Begin scaling analysis .... *
Declare Y8 as a tensor
for c1 in {core}:
 Read V2 from GA for cl
Declare X as a o^4 tensor
X_{()}(i,o3,k,o2) += 1.0 sum(o4,o1) D3(i,o3,k,o2,o4,o1) * Y8(o1,o4)
for c in {vir}:
 Read S2 from GA for c
```

```
eclipse_sort.dat
 9 11, 12 16:46
                                                                     Page 49/145
 Read T2 from GA for c
 S2_{(c)}(i,k,a) += -1 sum(03,02) T2(03,02,a,) * X_{(i,03,k,02)}
 Accumulate S2 (c)(i,k,a) for c
! No.15
! S2(i,k,a,c) <--
! ( -1.00000000) D3(i,o3,k,o2,o4,o1) T2(o2,o3,c,a) Y9(o1,o4)
Case 0 ..... X(i,k,o4,o1,c,a) <---- ( 1.00000000) D3(i,o3,k,o2,o4,o1) T2(o
! Polynomial order is O(o^6v^2)
! Maximum memory usage is O(o^4)
Case 1 ..... X(i,o3,k,o2) <---- ( 1.00000000) D3(i,o3,k,o2,o4,o1) Y9(o1,o4
! Polynomial order is O(o^4v^2)
! Maximum memory usage is O(o^4)
Case 2 ..... X(02,03,01,04,c,a) <---- ( 1.00000000) T2(02,03,c,a) Y9(01,04
! Polynomial order is O(o^6v^2)
! Maximum memory usage is O(o^4)
Factorize: Conflict between choices of optimal memory usage and polynomial order
! The optimal choice is .....
1: X(i,03,k,02) <-- ( 1.0000000) D3(i,03,k,02,04,01) Y9(01,04) 2: S2(i,k,a,c) <-- ( -1.00000000) T2(02,03,c,a) X(i,03,k,02)
               : O(o^4v^2)
! Max size of X : o^4
! * Begin scaling analysis .... *
Declare Y9 as a tensor
for c1 in {core}:
 Read V2 from GA for c1
Declare X as a o^4 tensor
X_{()}(i,o3,k,o2) += 1.0 sum(o4,o1) D3(i,o3,k,o2,o4,o1) * Y9(o1,o4)
for c in {vir}:
 Read S2 from GA for c
 for a in {vir}
   Read T2 from GA for a
   S2_{(c)}(i,k,a) += -1 sum(o2,o3) T2(o2,o3,c,) * X_{(i,o3,k,o2)}
    Accumulate S2_(c)(i,k,a) for c
! No.16
! S2(i,k,a,c) <--
! ( 2.00000000) D2(i,o2,k,o1) T2(o1,o2,v1,a) Y10(c,v1)
Case 0 ..... X(i,k,v1,a) < ---- (1.00000000) D2(i,o2,k,o1) T2(o1,o2,v1,a)
! Polynomial order is O(o^4v^2)
! Maximum memory usage is O(o^2v^1)
Case 1 ..... X(i,o2,k,o1,c,v1) < ---- (1.00000000) D2(i,o2,k,o1) Y10(c,v1)
! Polynomial order is O(o^4v^3)
! Maximum memory usage is O(o^4v^1)
Case 2 ..... X(o1,o2,a,c) <---- (
                                       1.00000000) T2(o1,o2,v1,a) Y10(c,v1)
! Polynomial order is O(o^4v^2)
! Maximum memory usage is O(o^2)
Factorize: Conflict between choices of optimal memory usage and polynomial order
```

9 11, 12 16:46	eclipse_sort.dat	Page 50/145
	 1.00000000) D2(i,o2,k,o1) 2.00000000) X(i,k,v1,a) Y10	
! Scaling : O(o^4v ! Max size of X : o^2v^1		
! * Begin scaling analys	is *	
Declare Y10 as a tensor for c1 in {core}: Read V2 from GA for c1		
<pre>for a in {vir}: Read T2 from GA for a Declare X as a o^2v^1 X_(a)(i,k,v1) += 1.0 s</pre>	tensor um(o2,o1) D2(i,o2,k,o1) * T2(o1,o2,v1,)
<pre>for c in {vir}: Read S2 from GA for S2_(c)(i,k,a) += 2 s</pre>	c um(v1) X_(a)(i,k,v1,) * Y10(c	·,v1)
Accumulate S2_(c)(i,	k,a) for c	
!		
! Indices of BareAmp are Case 0 X(i,k,v1,c) ! Polynomial order is O(! Maximum memory usage i		(i,o2,k,o1) T2(o2,o1,v1,c)
! Polynomial order is O(! Maximum memory usage i Case 2 X(o2,o1,c,a ! Polynomial order is O(! Maximum memory usage i	s O(o^4v^2) .) < (1.00000000) T o^4v^2)	2(o2,o1,v1,c) Y11(a,v1)
! The optimal choice is 1: X(i,k,v1,c) < (2: S2(i,k,a,c) < (1.00000000) D2(i,o2,k,o1) 2.00000000) X(i,k,v1,c) Y11	
! Scaling : O(o^4v ! Max size of X : o^2v^1		
! * Begin scaling analys	is *	
Declare Y11 as a tensor for c1 in {core}: Read V2 from GA for c1		
for c in {vir}: Read T2 from GA for c Read S2 from GA for c Declare X as a o^2v^1 X_(c)(i,k,v1) += 1.0 s	tensor um(o2,o1) D2(i,o2,k,o1) * T2(o2,o1,v1,)
S2_(c)(i,k,a) += 2 sum	(v1) X_(c)(i,k,v1,) * Y11(a,v	1)
Accumulate S2_(c)(i,k,	a) for c	

```
eclipse sort.dat
 9 11, 12 16:46
                                                                     Page 51/145
! S2(i,k,a,c) <--
! ( 2.00000000) D2(i,o2,k,o1) T2(o2,o1,a,v1) Y12(c,v1)
Case 0 ..... X(i,k,a,v1) < ---- (1.00000000) D2(i,o2,k,o1) T2(o2,o1,a,v1)
! Polynomial order is O(o^4v^2)
! Maximum memory usage is O(o^2v^1)
Case 1 ..... X(i,o2,k,o1,c,v1) <---- ( 1.00000000) D2(i,o2,k,o1) Y12(c,v1)
! Polynomial order is O(o^4v^3)
! Maximum memory usage is O(o^4)
Case 2 ..... X(02,01,a,c) < ---- (1.00000000) T2(02,01,a,v1) Y12(c,v1)
! Polynomial order is O(o^4v^2)
! Maximum memory usage is O(o^2v^1)
! The optimal choice is .....
1: X(i,k,a,v1) <-- ( 1.00000000) D2(i,o2,k,o1) T2(o2,o1,a,v1) 2: S2(i,k,a,c) <-- ( 2.00000000) X(i,k,a,v1) Y12(c,v1)
! Scaling
            : O(o^4v^2)
! Max size of X : o^2v^1
! * Begin scaling analysis .... *
Declare Y12 as a tensor
for c1 in {core}:
 Read V2 from GA for c1
for v1 in {vir}:
 Read T2 from GA for v1
 Declare X as a o^2v^1 tensor
 X(v1)(i,k,a) += 1.0 sum(o2,o1) D2(i,o2,k,o1) * T2(o2,o1,a,)
 for c in {vir}:
   Read S2 from GA for c
    S2(c)(i,k,a) += 2 sum() X (v1)(i,k,a,) * Y12(c,v1)
   Accumulate S2 (c)(i,k,a) for c
! No.19
! S2(i,k,a,c) <--
! ( 2.00000000) D2(i,o2,k,o1) T2(o1,o2,c,v1) Y13(a,v1)
Case 0 \dots X(i,k,c,v1) < ---- (1.00000000) D2(i,o2,k,o1) T2(o1,o2,c,v1)
! Polynomial order is O(o^4v^2)
! Maximum memory usage is O(o^2)
Case 1 ..... X(i,o2,k,o1,a,v1) < ---- (1.00000000) D2(i,o2,k,o1) Y13(a,v1)
! Polynomial order is O(o^4v^3)
! Maximum memory usage is O(o^4v^1)
Case 2 ..... X(o1,o2,c,a) < ---- (1.00000000) T2(o1,o2,c,v1) Y13(a,v1)
! Polynomial order is O(o^4v^2)
! Maximum memory usage is O(o^2v^1)
! The optimal choice is .....
1: X(i,k,c,v1) <-- ( 1.00000000) D2(i,o2,k,o1) T2(o1,o2,c,v1)
2: S2(i,k,a,c) <-- ( 2.00000000) X(i,k,c,v1) Y13(a,v1)
! Scaling
              : O(o^4v^2)
! Max size of X : o^2
! * Begin scaling analysis .... *
Declare Y13 as a tensor
```

```
eclipse sort.dat
  9 11, 12 16:46
                                                                     Page 52/145
for c1 in {core}:
  Read V2 from GA for cl
for c in {vir}:
  Read S2 from GA for c
  for v1 in {vir}:
   Read T2 from GA for v1
    Declare X as a o^2 tensor
    X(c,v1)(i,k) += 1.0 sum(o2,o1) D2(i,o2,k,o1) * T2(o1,o2,c,)
    S2(c)(i,k,a) += 2 sum() X(c,v1)(i,k,,) * Y13(a,v1)
    Accumulate S2 (c)(i,k,a) for c
! S2(i,k,a,c) <--
! ( -1.00000000) D2(i,o2,k,o1) T2(o1,o2,v1,a) Y14(c,v1)
Case 0 ..... X(i,k,v1,a) < ---- (1.00000000) D2(i,o2,k,o1) T2(o1,o2,v1,a)
! Polynomial order is O(o^4v^2)
! Maximum memory usage is O(o^2v^1)
Case 1 .... X(\hat{1},02,\bar{k},01,c,v1) < ---- ( 1.00000000) D2(i,02,k,01) Y14(c,v1)
! Polynomial order is O(o^4v^3)
! Maximum memory usage is O(o^4v^1)
Case 2 ..... X(o1,o2,a,c) < ---- (1.00000000) T2(o1,o2,v1,a) Y14(c,v1)
! Polynomial order is O(o^4v^2)
! Maximum memory usage is O(o^2)
Factorize: Conflict between choices of optimal memory usage and polynomial order
! The optimal choice is .....
1: X(i,k,vl,a) <-- ( 1.00000000) D2(i,o2,k,o1) T2(o1,o2,vl,a)

2: S2(i,k,a,c) <-- ( -1.00000000) X(i,k,vl,a) Y14(c,vl)
! Scaling
             : O(o^4v^2)
! Max size of X : o^2v^1
! * Begin scaling analysis .... *
Declare Y14 as a tensor
for c1 in {core}:
 Read V2 from GA for cl
for a in {vir}:
  Read T2 from GA for a
  Declare X as a o^2v^1 tensor
  X_{(a)}(i,k,v1) += 1.0 \text{ sum}(02,01) D2(i,02,k,01) * T2(01,02,v1,)
  for c in {vir}:
   Read S2 from GA for c
    S2_{(c)}(i,k,a) += -1 sum(v1) X_{(a)}(i,k,v1,) * Y14(c,v1)
    Accumulate S2_(c)(i,k,a) for c
! No.21
! S2(i,k,a,c) <--
! ( -1.00000000) D2(i,o2,k,o1) T2(o2,o1,v1,c) Y15(a,v1)
! Indices of BareAmp are rotated to match with LHS.
Case 0 ..... X(i,k,v1,c) < ---- ( 1.00000000) D2(i,o2,k,o1) T2(o2,o1,v1,c)
! Polynomial order is O(o^4v^2)
! Maximum memory usage is O(o^2v^1)
```

```
eclipse sort.dat
 9 11, 12 16:46
                                                                      Page 53/145
Case 1 .... X(i,o2,k,o1,a,v1) <---- ( 1.00000000) D2(i,o2,k,o1) Y15(a,v1)
! Polynomial order is O(o^4v^3)
! Maximum memory usage is O(o^4v^2)
Case 2 ..... X(02,01,c,a) < ---- ( 1.00000000) T2(02,01,v1,c) Y15(a,v1)
! Polynomial order is O(o^4v^2)
! Maximum memory usage is O(o^2v^1)
! The optimal choice is .....
1: X(i,k,v1,c) <-- ( 1.00000000) D2(i,o2,k,o1) T2(o2,o1,v1,c) 2: S2(i,k,a,c) <-- ( -1.00000000) X(i,k,v1,c) Y15(a,v1)
! Scaling : O(o^4v^2)
! Max size of X : o^2v^1
! * Begin scaling analysis .... *
Declare Y15 as a tensor
for c1 in {core}:
 Read V2 from GA for cl
for c in {vir}:
 Read T2 from GA for c
 Read S2 from GA for c
 Declare X as a o^2v^1 tensor
 X_{(c)(i,k,v1)} += 1.0 \text{ sum}(o2,o1) D2(i,o2,k,o1) * T2(o2,o1,v1,)
 S2(c)(i,k,a) += -1 sum(v1) X(c)(i,k,v1,) * Y15(a,v1)
 Accumulate S2 (c)(i,k,a) for c
! S2(i,k,a,c) <--
! ( -1.00000000) D2(i,o2,k,o1) T2(o2,o1,a,v1) Y16(c,v1)
Case 0 ..... X(i,k,a,v1) < ---- ( 1.00000000) D2(i,o2,k,o1) T2(o2,o1,a,v1)
! Polynomial order is O(o^4v^2)
! Maximum memory usage is O(o^2v^1)
Case 1 .... X(i,02,k,01,c,v1) < ---- ( 1.00000000) D2(i,02,k,01) Y16(c,v1)
! Polynomial order is O(o^4v^3)
! Maximum memory usage is O(o^4)
Case 2 .... X(o2,o1,a,c) <---- ( 1.00000000) T2(o2,o1,a,v1) Y16(c,v1)
! Polynomial order is O(o^4v^2)
! Maximum memory usage is O(o^2v^1)
! The optimal choice is .....
1: X(i,k,a,v1) < -- ( 1.00000000) D2(i,o2,k,o1) T2(o2,o1,a,v1) 2: S2(i,k,a,c) < -- ( -1.00000000) X(i,k,a,v1) Y16(c,v1)
! Scaling
              : O(o^4v^2)
! Max size of X : o^2v^1
! * Begin scaling analysis .... *
Declare Y16 as a tensor
for c1 in {core}:
 Read V2 from GA for c1
for v1 in {vir}:
 Read T2 from GA for v1
 Declare X as a o^2v^1 tensor
 X_{(v1)}(i,k,a) += 1.0 \text{ sum}(02,01) D2(i,02,k,01) * T2(02,01,a,)
 for c in {vir}:
   Read S2 from GA for c
```

```
eclipse sort.dat
  9 11, 12 16:46
                                                                    Page 54/145
    S2 (c)(i,k,a) += -1 sum() X (v1)(i,k,a,) * Y16(c,v1)
    Accumulate S2 (c)(i,k,a) for c
! No.23
! S2(i,k,a,c) <--
! (-1.00000000) D2(i,o2,k,o1) T2(o1,o2,c,v1) Y17(a,v1)
Case 0 ..... X(i,k,c,v1) < ---- ( 1.00000000) D2(i,o2,k,o1) T2(o1,o2,c,v1)
! Polynomial order is O(o^4v^2)
! Maximum memory usage is O(o^2)
Case 1 ..... X(i,o2,k,o1,a,v1) <---- ( 1.00000000) D2(i,o2,k,o1) Y17(a,v1)
! Polynomial order is O(o^4v^3)
! Maximum memory usage is O(o^4v^1)
Case 2 ..... X(o1,o2,c,a) < ---- (1.00000000) T2(o1,o2,c,v1) Y17(a,v1)
! Polynomial order is O(o^4v^2)
! Maximum memory usage is O(o^2v^1)
! The optimal choice is .....
1: X(i,k,c,v1) < -- ( 1.00000000) D2(i,o2,k,o1) T2(o1,o2,c,v1) 2: S2(i,k,a,c) < -- ( -1.00000000) X(i,k,c,v1) Y17(a,v1)
! Scaling : O(o^4v^2)
! Max size of X : o^2
! * Begin scaling analysis .... *
Declare Y17 as a tensor
for c1 in {core}:
 Read V2 from GA for c1
for c in {vir}:
  Read S2 from GA for c
  for v1 in {vir}:
    Read T2 from GA for v1
    Declare X as a o^2 tensor
    X_{(c,v1)(i,k)} += 1.0 \text{ sum}(02,01) D2(i,02,k,01) * T2(01,02,c,)
    S2 (c)(i,k,a) += -1 sum() X (c,v1)(i,k,,) * Y17(a,v1)
   Accumulate S2_(c)(i,k,a) for c
1 No. 24
! S2(i,k,a,c) <--
! (0.50000000) D4(i,o4,k,o3,o5,o1,o6,o2) T2(o4,o3,a,c) V2(o1,o5,o2,o6)
! Indices of BareAmp are rotated to match with LHS.
! Indices of ERI and D4 are rotated to match with each other.
H2: 0 D4: 25
*TEST* ( 0.50000000) D4(o1,o5,o4,i,o3,k,o2,o6) T2(o4,o3,a,c) V2(o1,o5,o2,o6)
! *** D4(01,05,04,i,03,k,02,06) T2(04,03,a,c) is skipped due to the priority
Case 1 .... X(04,i,03,k) < ---- ( 1.00000000) D4(01,05,04,i,03,k,02,06) V2
(01,05,02,06)
! Polynomial order is O(o^8)
! Maximum memory usage is O(o^4)
Case 2 .... X(04,03,01,05,02,06,a,c) <---- ( 1.00000000) T2(04,03,a,c) V2
(01,05,02,06)
! Polynomial order is O(o^8v^2)
! Maximum memory usage is O(o^4v^1)
! The optimal choice is .....
1: X(04, 1, 03, k) < -- ( 1.00000000) D4(01, 05, 04, 1, 03, k, 02, 06) V2(01, 05, 02, 06)
```

```
eclipse sort.dat
 9 11, 12 16:46
                                                                  Page 55/145
2: S2(i,k,a,c) < -- ( 0.50000000) T2(04,03,a,c) X(04,i,03,k)
             : O(o^8)
! Max size of X : o^4
! * Begin scaling analysis .... *
! Intermediate is not processed in ad hoc fashion ....
Declare X as a o^4 tensor
for ol in {occ}:
 Read V2 from GA for ol
 for o5 in {occ}:
   Read D4 from GA for o1,05
   X()(04,i,03,k) += 1.0 sum(02,06) V2(,05,02,06) * D4(,,04,i,03,k,02,06)
for c in {vir}:
 Read S2 from GA for c
 Read T2 from GA for c
 S2(c)(i,k,a) += 0.5 sum(04,03) T2(04,03,a,) * X()(04,i,03,k)
 Accumulate S2 (c)(i,k,a) for c
! No.25
! S2(i,k,a,c) <--
! (0.50000000) D4(i,o3,k,o4,o1,o5,o2,o6) T2(o4,o3,c,a) V2(o1,o5,o2,o6)
! Indices of ERI and D4 are rotated to match with each other.
H2: 0 D4: 24
*TEST* ( 0.50000000) D4(o1,o5,i,o3,k,o4,o2,o6) T2(o4,o3,c,a) V2(o1,o5,o2,o6)
! *** D4(01,05,i,03,k,04,02,06) T2(04,03,c,a) is skipped due to the priority
Case 1 .... X(i,o3,k,o4) < ---- ( 1.00000000) D4(o1,o5,i,o3,k,o4,o2,o6) V2
(01,05,02,06)
! Polynomial order is O(o^8)
! Maximum memory usage is O(o^4)
Case 2 ..... X(04.03.01.05.02.06.c.a) <---- ( 1.00000000) T2(04.03.c.a) V2
(01,05,02,06)
! Polynomial order is O(o^8v^2)
! Maximum memory usage is O(o^4)
! The optimal choice is .....
1: X(i,03,k,04) < -- (1.00000000) D4(01,05,i,03,k,04,02,06) V2(01,05,02,06
2: S2(i,k,a,c) < -- (0.50000000) T2(04,03,c,a) X(i,03,k,04)
! Scaling
             : O(o^8)
! Max size of X : o^4
! * Begin scaling analysis .... *
! Intermediate is not processed in ad hoc fashion ....
Declare X as a o^4 tensor
for o1 in {occ}:
 Read V2 from GA for ol
 for o5 in {occ}:
   Read D4 from GA for ol.o5
   X_{()}(i,03,k,04) += 1.0 sum(02,06) V2(,05,02,06) * D4(,,i,03,k,04,02,06)
for c in {vir}:
 Read S2 from GA for c
 for a in {vir}
   Read T2 from GA for a
   S2_{(c)}(i,k,a) += 0.5 \text{ sum}(04,03) T2(04,03,c,) * X_{(i,03,k,04)}
```

```
eclipse sort.dat
                                                                      Page 56/145
  9 11, 12 16:46
    Accumulate S2 (c)(i,k,a) for c
! No.26
! S2(i,k,a,c) <--
! ( 1.00000000) D3(i,o3,k,o2,o4,o1) T2(o2,o3,v1,a) V2(o1,o4,c,v1)
! Indices of ERI are rotated to match with LHS.
! *** D3(i,o3,k,o2,o4,o1) T2(o2,o3,v1,a) is skipped due to the priority
Case 1 ..... X(i,o3,k,o2,c,v1) < ---- ( 1.00000000) D3(i,o3,k,o2,o4,o1) V2(
c,v1,o1,o4)
! Polynomial order is O(o^6v^2)
! Maximum memory usage is O(o^4v^1)
Case 2 ..... X(02,03,01,04,a,c) <---- ( 1.00000000) T2(02,03,v1,a) V2(c,v1
,01,04)
! Polynomial order is O(o^6v^2)
! Maximum memory usage is O(o^4)
Factorize: Conflict between choices of optimal memory usage and polynomial order
! The optimal choice is .....
1: X(i,o3,k,o2,c,v1) <-- ( 1.00000000) D3(i,o3,k,o2,o4,o1) V2(c,v1,o1,o4) 
2: S2(i,k,a,c) <-- ( 1.00000000) T2(o2,o3,v1,a) X(i,o3,k,o2,c,v1)
! Scaling
              : O(o^6v^2)
! Max size of X : o^4v^1
! * Begin scaling analysis .... *
for c in {vir}:
  Read V2 from GA for c
  Read S2 from GA for c
  Declare X as a o^4v^1 tensor
  X_{(c)}(i,o3,k,o2,v1) += 1.0 sum(o1,o4) V2(,v1,o1,o4) * D3(i,o3,k,o2,o4,o1)
  for a in {vir}
    Read T2 from GA for a
    S2(c)(i,k,a) += 1.0 sum(o2.o3.v1) T2(o2.o3.v1.) * X(c)(i,o3.k.o2..v1)
    Accumulate S2_(c)(i,k,a) for c
! No.27
! S2(i,k,a,c) <--
! ( 1.00000000) D3(i,o3,k,o2,o4,o1) T2(o3,o2,v1,c) V2(o1,o4,a,v1)
! Indices of BareAmp are rotated to match with LHS.
! The indices of ERI are rotated to became virtual.
! *** D3(i,o3,k,o2,o4,o1) T2(o3,o2,v1,c) is skipped due to the priority
Case 1 .... X(i,o3,k,o2,a,v1) < ---- ( 1.00000000) D3(i,o3,k,o2,o4,o1) V2(
a.v1.o1.o4)
! Polynomial order is O(o^6v^2)
! Maximum memory usage is O(o^4v^1)
Case 2 ..... X(03,02,01,04,c,a) <---- ( 1.00000000) T2(03,02,v1,c) V2(a,v1
,01,04)
! Polynomial order is O(o^6v^2)
! Maximum memory usage is O(o^4)
Factorize: Conflict between choices of optimal memory usage and polynomial order
! The optimal choice is .....
1: X(i,o3,k,o2,a,v1) <-- ( 1.00000000) D3(i,o3,k,o2,o4,o1) V2(a,v1,o1,o4) 
2: S2(i,k,a,c) <-- ( 1.00000000) T2(o3,o2,v1,c) X(i,o3,k,o2,a,v1)
! Scaling
                : O(o^6v^2)
```

```
eclipse sort.dat
 9 11, 12 16:46
                                                                      Page 57/145
! Max size of X : o^4v^1
! * Begin scaling analysis .... *
for a in {vir}:
 Read V2 from GA for a
 Declare X as a o^4v^1 tensor
 X_{(a)}(i,o3,k,o2,v1) += 1.0 sum(o1,o4) V2(,v1,o1,o4) * D3(i,o3,k,o2,o4,o1)
 for c in {vir}:
    Read S2 from GA for c
    Read T2 from GA for c
    S2(c)(i,k,a) += 1.0 sum(o3,o2,v1) T2(o3,o2,v1,) * X(a)(i,o3,k,o2,v1)
    Accumulate S2_(c)(i,k,a) for c
! No.28
! S2(i,k,a,c) <--
      1.00000000) D3(i,o3,k,o2,o4,o1) T2(o3,o2,a,v1) V2(o1,o4,c,v1)
! Indices of ERI are rotated to match with LHS.
! *** D3(i,o3,k,o2,o4,o1) T2(o3,o2,a,v1) is skipped due to the priority
Case 1 ..... X(i,o3,k,o2,c,v1) <---- ( 1.00000000) D3(i,o3,k,o2,o4,o1) V2(
c,v1,o1,o4)
! Polynomial order is O(o^6v^2)
! Maximum memory usage is O(o^4)
Case 2 ..... X(03,02,01,04,a,c) <---- ( 1.00000000) T2(03,02,a,v1) V2(c,v1
,01,04)
! Polynomial order is O(o^6v^2)
! Maximum memory usage is O(o^4v^1)
! The optimal choice is .....
1: X(i,o3,k,o2,c,v1) <-- ( 1.00000000) D3(i,o3,k,o2,o4,o1) V2(c,v1,o1,o4) 
2: S2(i,k,a,c) <-- ( 1.00000000) T2(o3,o2,a,v1) X(i,o3,k,o2,c,v1)
! Scaling
              : O(o^6v^2)
! Max size of X : o^4
! * Begin scaling analysis .... *
for c in {vir}:
 Read V2 from GA for c
 Read S2 from GA for c
 for v1 in {vir}:
   Read T2 from GA for v1
    Declare X as a o^4 tensor
   X_{(c,v1)}(i,o3,k,o2) += 1.0 sum(o1,o4) V2(,v1,o1,o4) * D3(i,o3,k,o2,o4,o1)
    S2_{(c)}(i,k,a) += 1.0 sum(03,02) T2(03,02,a,) * X_{(c,v1)}(i,03,k,02,,)
   Accumulate S2_(c)(i,k,a) for c
! No.29
! S2(i,k,a,c) <--
! (1.00000000) D3(i,o2,k,o3,o1,o4) T2(o3,o2,c,v1) V2(o1,o4,a,v1)
! Indices of ERI are rotated to match with Bareamp.
! *** D3(i,o2,k,o3,o1,o4) T2(o3,o2,c,v1) is skipped due to the priority
Case 1 ..... X(i,o2,k,o3,v1,a) < ---- (1.00000000) D3(i,o2,k,o3,o1,o4) V2(i,o2,k,o3,o1,o4)
v1,a,o1,o4)
! Polynomial order is O(o^6v^2)
! Maximum memory usage is O(o^4v^1)
Case 2 ..... X(03,02,01,04,c,a) < ---- ( 1.00000000) T2(03,02,c,v1) V2(v1,a)
```

```
eclipse sort.dat
  9 11, 12 16:46
                                                                        Page 58/145
 ,01,04)
 ! Polynomial order is O(o^6v^2)
! Maximum memory usage is O(o^4v^1)
 ! The optimal choice is .....
1: X(i,o_2,k,o_3,v_1,a) < -- (1.00000000) D3(i,o_2,k,o_3,o_1,o_4) V2(v_1,a,o_1,o_4)
2: S2(i,k,a,c) <-- ( 1.00000000) T2(03,02,c,v1) X(i,02,k,03,v1,a)
! Scaling
               : O(o^6v^2)
! Max size of X : o^4v^1
! * Begin scaling analysis .... *
for v1 in {vir}:
  Read V2 from GA for v1
  Read T2 from GA for v1
  Declare X as a o^4v^1 tensor
  X_{v1}(v1)(i,o2,k,o3,a) += 1.0 sum(o1,o4) V2(,a,o1,o4) * D3(i,o2,k,o3,o1,o4)
  for c in {vir}:
    Read S2 from GA for c
    S2_{(c)}(i,k,a) += 1.0 sum(03,02) T2(03,02,c,) * X_{(v1)}(i,02,k,03,a)
    Accumulate S2 (c)(i,k,a) for c
! No.30
! S2(i,k,a,c) <--
! ( 1.00000000) D3(i,o3,k,o2,o4,o1) T2(o1,o3,v1,a) V2(o2,c,o4,v1)
! Indices of ERI are rotated to match with LHS.
! *** D3(i,o3,k,o2,o4,o1) T2(o1,o3,v1,a) is skipped due to the priority
Case 1 ..... X(i,o3,k,o1,c,v1) < ---- (1.00000000) D3(i,o3,k,o2,o4,o1) V2(
c,o2,o4,v1)
! Polynomial order is O(o^6v^2)
! Maximum memory usage is O(o^4v^1)
Case 2 ..... X(o1,o3,o2,o4,a,c) <---- ( 1.00000000) T2(o1,o3,v1,a) V2(c,o2
.04.v1)
! Polynomial order is O(o^6v^2)
! Maximum memory usage is O(o^4)
Factorize: Conflict between choices of optimal memory usage and polynomial order
! The optimal choice is .....
1: X(i,o3,k,o1,c,v1) <-- ( 1.00000000) D3(i,o3,k,o2,o4,o1) V2(c,o2,o4,v1)
2: S2(i,k,a,c) <-- ( 1.00000000) T2(o1,o3,v1,a) X(i,o3,k,o1,c,v1)
! Scaling
               : O(o^6v^2)
! Max size of X : o^4v^1
! * Begin scaling analysis .... *
for c in {vir}:
  Read V2 from GA for c
  Read S2 from GA for c
  Declare X as a o^4v^1 tensor
  X_{(c)}(i,o3,k,o1,v1) += 1.0 sum(o2,o4) V2(,o2,o4,v1) * D3(i,o3,k,o2,o4,o1)
  for a in {vir}
    Read T2 from GA for a
    S2_{(c)}(i,k,a) += 1.0 \text{ sum}(01,03,v1) T2(01,03,v1,) * X_{(c)}(i,03,k,01,v1)
    Accumulate S2_(c)(i,k,a) for c
```

```
eclipse sort.dat
 9 11, 12 16:46
                                                                         Page 59/145
! No.31
! S2(i,k,a,c) <--
! (1.00000000) D3(i,o3,k,o2,o4,o1) T2(o1,o2,v1,c) V2(o3,a,o4,v1)
! Indices of BareAmp are rotated to match with LHS.
! The indices of ERI are rotated to became virtual.
! *** D3(i,o3,k,o2,o4,o1) T2(o1,o2,v1,c) is skipped due to the priority
Case 1 .... X(i,k,o2,o1,a,v1) <---- ( 1.00000000) D3(i,o3,k,o2,o4,o1) V2(
a, o3, o4, v1)
! Polynomial order is O(o^6v^2)
! Maximum memory usage is O(o^4v^1)
Case 2 ..... X(o1,o2,o3,o4,c,a) <---- ( 1.00000000) T2(o1,o2,v1,c) V2(a,o3
,o4,v1)
! Polynomial order is O(o^6v^2)
! Maximum memory usage is O(o^4)
Factorize: Conflict between choices of optimal memory usage and polynomial order
! The optimal choice is .....
1: X(i,k,o2,o1,a,v1) <-- ( 1.00000000) D3(i,o3,k,o2,o4,o1) V2(a,o3,o4,v1)
2: S2(i,k,a,c) <-- ( 1.00000000) T2(o1,o2,v1,c) X(i,k,o2,o1,a,v1)
              : O(o^6v^2)
! Max size of X : o^4v^1
! * Begin scaling analysis .... *
for a in {vir}:
 Read V2 from GA for a
  Declare X as a o^4v^1 tensor
  X (a)(i,k,o2,o1,v1) += 1.0 sum(o3,o4) V2(,o3,o4,v1) * D3(i,o3,k,o2,o4,o1)
  for c in {vir}:
    Read S2 from GA for c
    Read T2 from GA for c
    S2_{(c)}(i,k,a) += 1.0 sum(o1,o2,v1) T2(o1,o2,v1,) * X_{(a)}(i,k,o2,o1,,v1)
    Accumulate S2 (c)(i,k,a) for c
! No.32
! S2(i,k,a,c) <--
! ( 1.00000000) D3(i,o3,k,o2,o4,o1) T2(o3,o1,a,v1) V2(o2,c,o4,v1)
! Indices of ERI are rotated to match with LHS.
! *** D3(i,o3,k,o2,o4,o1) T2(o3,o1,a,v1) is skipped due to the priority
Case 1 .... X(i,o3,k,o1,c,v1) <---- ( 1.00000000) D3(i,o3,k,o2,o4,o1) V2(
c,o2,o4,v1)
! Polynomial order is O(o^6v^2)
! Maximum memory usage is O(o^4)
Case 2 .... X(03,01,02,04,a,c) <---- ( 1.00000000) T2(03,01,a,v1) V2(c,02
,o4,v1)
! Polynomial order is O(o^6v^2)
! Maximum memory usage is O(o^4v^1)
! The optimal choice is .....
1: X(i,o3,k,o1,c,v1) <-- ( 1.00000000) D3(i,o3,k,o2,o4,o1) V2(c,o2,o4,v1)
2: S2(i,k,a,c) <-- ( 1.00000000) T2(o3,o1,a,v1) X(i,o3,k,o1,c,v1)
! Scaling
               : O(o^6v^2)
! Max size of X : o^4
! * Begin scaling analysis .... *
for c in {vir}:
 Read V2 from GA for c
  Read S2 from GA for c
```

```
eclipse sort.dat
                                                                     Page 60/145
  9 11, 12 16:46
  for v1 in {vir}:
    Read T2 from GA for v1
    Declare X as a o^4 tensor
    X(c,v1)(i,o3,k,o1) += 1.0 sum(o2,o4) V2(,o2,o4,v1) * D3(i,o3,k,o2,o4,o1)
    S2_{(c)(i,k,a)} += 1.0 sum(o3,o1) T2(o3,o1,a,) * X_{(c,v1)(i,o3,k,o1,,)}
    Accumulate S2_(c)(i,k,a) for c
! No.33
! S2(i,k,a,c) <--
! ( 1.00000000) D3(i,o2,k,o3,o1,o4) T2(o3,o4,c,v1) V2(o1,v1,o2,a)
! Indices of ERI are rotated to match with Bareamp.
! *** D3(i,o2,k,o3,o1,o4) T2(o3,o4,c,v1) is skipped due to the priority
Case 1 ..... X(i,k,o3,o4,v1,a) < ---- (1.00000000) D3(i,o2,k,o3,o1,o4) V2(i,b,o3,o1,o4)
v1,o1,o2,a)
! Polynomial order is O(o^6v^2)
! Maximum memory usage is O(o^4v^1)
Case 2 ..... X(03,04,01,02,c,a) <---- ( 1.00000000) T2(03,04,c,v1) V2(v1,0
1,o2,a)
! Polynomial order is O(o^6v^2)
! Maximum memory usage is O(o^4v^1)
! The optimal choice is .....
1: X(i,k,o3,o4,v1,a) <-- ( 1.00000000) D3(i,o2,k,o3,o1,o4) V2(v1,o1,o2,a) 
2: S2(i,k,a,c) <-- ( 1.00000000) T2(o3,o4,c,v1) X(i,k,o3,o4,v1,a)
               : O(o^6v^2)
! Max size of X : o^4v^1
! * Begin scaling analysis .... *
for v1 in {vir}:
  Read V2 from GA for v1
  Read T2 from GA for v1
  Declare X as a o^4v^1 tensor
  X_{(v1)(i,k,o3,o4,a)} += 1.0 sum(o1,o2) V2(,o1,o2,a) * D3(i,o2,k,o3,o1,o4)
  for c in {vir}:
   Read S2 from GA for c
    S2_{(c)}(i,k,a) += 1.0 sum(03,04) T2(03,04,c,) * X_{(v1)}(i,k,03,04,a)
    Accumulate S2_(c)(i,k,a) for c
! No.34
! S2(i,k,a,c) <--
! ( 1.00000000) D2(i,o1,k,o2) T2(o1,o2,v1,v2) V2(a,v1,c,v2)
! Indices of ERI are rotated to match with LHS.
! *** D2(i,o1,k,o2) T2(o1,o2,v1,v2) is skipped due to the priority
Case 1 ..... X(i,o1,k,o2,c,v2,a,v1) <---- ( 1.00000000) D2(i,o1,k,o2) V2(c
.v2.a.v1)
! Polynomial order is O(o^4v^4)
! Maximum memory usage is O(o^4v^2)
Case 2 ..... X(o1,o2,c,a) < ---- (1.00000000) T2(o1,o2,v1,v2) V2(c,v2,a,v1)
! Polynomial order is O(o^2v^4)
! Maximum memory usage is O(o^2v^1)
! The optimal choice is .....
1: X(o1,o2,c,a) <-- ( 1.00000000) T2(o1,o2,v1,v2) V2(c,v2,a,v1)
2: S2(i,k,a,c) < -- ( 1.00000000) D2(i,o1,k,o2) X(o1,o2,c,a)
```

```
eclipse_sort.dat
                                                                        Page 61/145
  9 11, 12 16:46
! Scaling
              : O(o^2v^4)
! Max size of X : o^2v^1
! * Begin scaling analysis .... *
for c in {vir}:
 Read V2 from GA for c
  Read S2 from GA for c
  Declare X as a o^2v^1 tensor
  for v2 in {vir}:
    Read T2 from GA for v2
    X_{(c)}(o1,o2,a) += 1.0 sum(v1) V2(,v2,a,v1) * T2(o1,o2,v1,)
  S2_{(c)}(i,k,a) += 1.0 sum(o1,o2) D2(i,o1,k,o2) * X_{(c)}(o1,o2,,a)
  Accumulate S2 (c)(i,k,a) for c
! S2(i,k,a,c) <--
! ( 1.00000000) D2(i,o1,k,o2) T2(o2,o1,v1,v2) V2(a,v2,c,v1)
! Indices of ERI are rotated to match with LHS.
! *** D2(i,o1,k,o2) T2(o2,o1,v1,v2) is skipped due to the priority
Case 1 ..... X(i,o1,k,o2,c,v1,a,v2) <---- ( 1.00000000) D2(i,o1,k,o2) V2(c
,v1,a,v2)
! Polynomial order is O(o^4v^4)
! Maximum memory usage is O(o^4v^2)
Case 2 ..... X(o2,o1,c,a) <---- ( 1.00000000) T2(o2,o1,v1,v2) V2(c,v1,a,v2
! Polynomial order is O(o^2v^4)
! Maximum memory usage is O(o^2v^1)
! The optimal choice is .....
1: X(o2,o1,c,a) <-- ( 1.00000000) T2(o2,o1,v1,v2) V2(c,v1,a,v2) 2: S2(i,k,a,c) <-- ( 1.00000000) D2(i,o1,k,o2) X(o2,o1,c,a)
! Scaling
                 : O(o^2v^4)
! Max size of X : o^2v^1
! * Begin scaling analysis .... *
for c in {vir}:
  Read V2 from GA for c
  Read S2 from GA for c
  Declare X as a o^2v^1 tensor
 for v2 in {vir}:
    Read T2 from GA for v2
    X_{(c)}(o2,o1,a) += 1.0 sum(v1) V2(,v1,a,v2) * T2(o2,o1,v1,)
  S2_{(c)}(i,k,a) += 1.0 sum(o1,o2) D2(i,o1,k,o2) * X_{(c)}(o2,o1,a)
  Accumulate S2_(c)(i,k,a) for c
* 2 <oovv/ooov>
     \begin{array}{lll} 0.50000000) & T2(\texttt{o1},\texttt{o2},\texttt{o3},\texttt{a}) & V2(\texttt{c1},\texttt{o4},\texttt{c2},\texttt{c}) & E4(\texttt{c1},\texttt{i},\texttt{k},\texttt{o3},\texttt{c2},\texttt{o2},\texttt{o4},\texttt{o1}) \\ 0.50000000) & T2(\texttt{o1},\texttt{o2},\texttt{o3},\texttt{c}) & V2(\texttt{c1},\texttt{o4},\texttt{c2},\texttt{a}) & E4(\texttt{c1},\texttt{i},\texttt{k},\texttt{o3},\texttt{c2},\texttt{o4},\texttt{o2},\texttt{o1}) \end{array}
      0.50000000) T2(o1,o2,o3,a) V2(c1,o3,c2,c) E3(c1,i,k,c2,o2,o1)
      0.50000000) T2(o1,o2,o3,c) V2(c1,o3,c2,a) E3(c1,i,k,c2,o1,o2)
      0.50000000) T2(o1,o2,o3,a) V2(c1,c2,o4,c) E4(c1,i,k,o3,o4,o2,c2,o1)
      0.50000000) T2(01,02,03,C) V2(c1,c2,04,a) E4(c1,i,k,03,04,c2,02,01)
```

```
eclipse sort.dat
   9 11, 12 16:46
                                                                                     Page 62/145
       0.50000000) T2(o1,o2,o3,a) V2(c1,c2,o3,c) E3(c1,i,k,o1,o2,c2)
       0.50000000) T2(o1,o2,o3,c) V2(c1,c2,o3,a) E3(c1,i,k,o1,c2,o2)
       0.50000000) T2(01,02,03,a) V2(04,06,05,c) E4(i,k,03,04,02,06,01,05)
       0.50000000) T2(o1,o2,o3,c) V2(o4,o6,o5,a) E4(i,k,o3,o4,o6,o2,o1,o5)
       0.50000000) T2(o1,o2,o3,a) V2(o3,o5,o4,c) E3(i,k,o4,o2,o5,o1)
       0.50000000) T2(o1,o2,o3,c) V2(o3,o5,o4,a) E3(i,k,o4,o5,o2,o1)
       0.50000000) T2(o1,o2,o3,a) V2(o3,o4,c,o5) E3(i,k,o4,o2,o1,o5)
       0.50000000) T2(o1,o2,o3,c) V2(o3,o4,a,o5) E3(i,k,o4,o1,o2,o5)
      0.50000000) T2(o1,o2,o3,a) V2(c1,c2,o4,c) E4(c1,i,k,o3,o4,o2,c2,o1) 0.50000000) T2(o1,o2,o3,c) V2(c1,c2,o4,a) E4(c1,i,k,o3,o4,c2,o2,o1)
       0.50000000) T2(o1,o2,o3,a) V2(c1,c2,o3,c) E3(c1,i,k,o1,o2,c2)
       0.50000000) T2(o1,o2,o3,c) V2(c1,c2,o3,a) E3(c1,i,k,o1,c2,o2)
      0.50000000) T2(o1,o2,o3,a) V2(c1,o4,c2,c) E4(c1,i,k,o3,c2,o2,o4,o1) 0.50000000) T2(o1,o2,o3,c) V2(c1,o4,c2,a) E4(c1,i,k,o3,c2,o4,o2,o1)
      0.50000000) T2(o1,o2,o3,a) V2(c1,o3,c2,c) E3(c1,i,k,c2,o2,o1) 0.50000000) T2(o1,o2,o3,c) V2(c1,o3,c2,a) E3(c1,i,k,c2,o1,o2)
       0.50000000) T2(o1,o2,o3,a) V2(o4,o5,o6,c) E4(i,k,o3,o4,o2,o5,o1,o6)
       0.50000000) T2(01,02,03,c) V2(04,05,06,a) E4(i,k,03,04,05,02,01,06)
       0.50000000) T2(o1,o2,o3,a) V2(o3,o5,o4,c) E3(i,k,o4,o2,o5,o1)
       0.50000000) T2(o1,o2,o3,c) V2(o3,o5,o4,a) E3(i,k,o4,o5,o2,o1)
      0.50000000) T2(o1,o2,o3,a) V2(o3,o4,c,o5) E3(i,k,o4,o2,o1,o5) 0.50000000) T2(o1,o2,o3,a) V2(o3,o4,a,o5) E3(i,k,o4,o2,o1,o5) 0.50000000) T2(o1,o2,o3,v1) V2(o4,c,a,v1) E3(i,k,o3,o4,o2,o1) 0.50000000) T2(o1,o2,o3,v1) V2(o4,c,a,v1) E3(i,k,o3,o4,o2,o1) 0.50000000) T2(o1,o2,o3,v1) V2(o4,a,c,v1) E3(i,k,o3,o2,o4,o1)
      0.50000000) T2(o1,o2,o3,v1) V2(o3,c,a,v1) E2(i,k,o1,o2) 0.50000000) T2(o1,o2,o3,v1) V2(o3,a,c,v1) E2(i,k,o2,o1)
       0.50000000) T2(o1,o2,o3,v1) V2(o4,a,c,v1) E3(i,k,o3,o2,o4,o1)
       0.50000000) T2(o1,o2,o3,v1) V2(o4,c,a,v1) E3(i,k,o3,o4,o2,o1)
       0.50000000) T2(o1,o2,o3,v1) V2(o3,a,c,v1) E2(i,k,o2,o1)
       0.50000000) T2(o1,o2,o3,v1) V2(o3,c,a,v1) E2(i,k,o1,o2)
Decompose RDMs .....
< RESULT >
                 1.00000000) D3(i,k,o4,o3,o2,o1) T2(o1,o3,o4,a) h(o2,c)
     0 : (
     1: (
                 1.00000000) D3(i,k,o1,o2,o3,o4) T2(o4,o3,o1,c) h(o2,a)
    2: (
                 1.00000000) D2(i,k,o3,o2) T2(o2,o3,o1,a) h(o1,c)
   3 : (
4 : (
5 : (
                 1.00000000) D2(i,k,o1,o2) T2(o1,o2,o3,c) h(o3,a)
                 2.00000000) D3(i,k,o4,o3,o2,o1) T2(o1,o3,o4,a) V2(c1,o2,c1,c) 2.00000000) D3(i,k,o4,o3,o2,o1) T2(o1,o2,o4,c) V2(c1,o3,c1,a)
     6 : (
                 2.00000000) D2(i,k,o3,o2) T2(o2,o3,o1,a) V2(c1,o1,c1,c)
     7 : ( 2.00000000) D2(i,k,o3,o2) T2(o3,o2,o1,c) V2(c1,o1,c1,a)
    8: (-1.00000000) D3(i,k,04,03,02,01) T2(01,03,04,a) V2(c1,c1,02,c)
    9: ( -1.00000000) D3(i,k,o4,o3,o2,o1) T2(o1,o2,o4,c) V2(c1,c1,o3,a)

10: ( -1.00000000) D2(i,k,o3,o2) T2(o2,o3,o1,a) V2(c1,c1,o1,c)

11: ( -1.00000000) D2(i,k,o3,o2) T2(o3,o2,o1,c) V2(c1,c1,o1,a)
    12: (
               1.00000000) D4(i,k,o6,o5,o4,o3,o2,o1) T2(o2,o4,o6,a) V2(o5,o3,o1,c)
    13 : (1.00000000) D4(i,k,o1,o2,o3,o4,o5,o6) T2(o5,o4,o1,c) V2(o2,o3,o6,a)
   14 : (
15 : (
16 : (
                1.00000000) D3(i,k,o5,o4,o3,o2) T2(o2,o4,o1,a) V2(o5,o3,o1,c) 1.00000000) D3(i,k,o5,o4,o3,o2) T2(o2,o3,o1,c) V2(o5,o4,o1,a)
                 1.00000000) D3(i,k,o5,o4,o3,o2) T2(o3,o4,o1,a) V2(o5,o1,o2,c)
  17 : (
                 1.00000000) D3(i,k,o5,o4,o3,o2) T2(o4,o3,o1,c) V2(o5,o1,o2,a)
   18 : (
                 1.00000000) D3(i,k,o1,o2,o3,o4) T2(o4,o3,o1,v1) V2(o2,c,a,v1)
    19 : (
                 1.00000000) D3(i,k,o1,o2,o3,o4) T2(o4,o2,o1,v1) V2(o3,a,c,v1)
    20 : (
                 1.00000000) D2(i,k,o1,o2) T2(o1,o2,o3,v1) V2(o3,c,a,v1)
    21 : (
                 1.00000000) D2(i,k,o1,o2) T2(o2,o1,o3,v1) V2(o3,a,c,v1)
< RESULT2 >
    0 : (
                1.00000000) D3(i,o3,k,o2,o4,o1) T2(o1,o3,o4,a) h(o2,c)
  1 : (
2 : (
3 : (
                 1.00000000) D3(i,o2,k,o3,o1,o4) T2(o4,o3,o1,c) h(o2,a)
                1.00000000) D2(i,o3,k,o2) T2(o2,o3,o1,a) h(o1,c) 1.00000000) D2(i,o1,k,o2) T2(o1,o2,o3,c) h(o3,a)
    4 : (
                 2.00000000) D3(i,o3,k,o2,o4,o1) T2(o1,o3,o4,a) V2(c1,c1,o2,c)
    5 : (
                 2.00000000) D3(i,o3,k,o2,o4,o1) T2(o1,o2,o4,c) V2(c1,c1,o3,a)
```

2.00000000) D2(i,o3,k,o2) T2(o2,o3,o1,a) V2(c1,c1,o1,c)

6 : (

```
eclipse_sort.dat
 9 11, 12 16:46
                                                                   Page 63/145
    7: (
             2.00000000) D2(i,o3,k,o2) T2(o3,o2,o1,c) V2(c1,c1,o1,a)
            -1.00000000) D3(i,o3,k,o2,o4,o1) T2(o1,o3,o4,a) V2(c1,o2,c1,c)
   8: (
    9: (
            -1.00000000) D3(i,o3,k,o2,o4,o1) T2(o1,o2,o4,c) V2(c1,o3,c1,a)
   10: (
            -1.00000000) D2(i,o3,k,o2) T2(o2,o3,o1,a) V2(c1,o1,c1,c)
            -1.00000000) D2(i,o3,k,o2) T2(o3,o2,o1,c) V2(c1,o1,c1,a)
   11: (
   12: ( 1.00000000) D4(i,o4,k,o3,o5,o1,o6,o2) T2(o2,o4,o6,a) V2(o1,o5,o3,c)
   13 : (
             1.00000000) D4(i,03,k,04,01,05,02,06) T2(05,04,01,c) V2(02,06,03,a)
             1.00000000) D3(i,o4,k,o3,o5,o2) T2(o2,o4,o1,a) V2(o1,o5,o3,c)
             1.00000000) D3(i,o4,k,o3,o5,o2) T2(o2,o3,o1,c) V2(o1,o5,o4,a)
   15 : (
   16: (
             1.00000000) D3(i,o4,k,o3,o5,o2) T2(o3,o4,o1,a) V2(o1,c,o2,o5)
   17: (
             1.00000000) D3(i,o4,k,o3,o5,o2) T2(o4,o3,o1,c) V2(o1,a,o2,o5)
             1.00000000) D3(i,o2,k,o3,o1,o4) T2(o4,o3,o1,v1) V2(o2,a,c,v1)
   18: (
   19: (
             1.00000000) D3(i,o2,k,o3,o1,o4) T2(o4,o2,o1,v1) V2(o3,c,a,v1)
   20 : (
             1.00000000) D2(i,o1,k,o2) T2(o1,o2,o3,v1) V2(o3,a,c,v1) 1.00000000) D2(i,o1,k,o2) T2(o2,o1,o3,v1) V2(o3,c,a,v1)
  21 : (
            1.00000000) D3(i,o3,k,o2,o4,o1) T2(o1,o3,o4,a) h(o2,c)
   0 : (
    1: (
             1.00000000) D3(i,o2,k,o3,o1,o4) T2(o4,o3,o1,c) h(o2,a)
    2: (
             1.00000000) D2(i,o3,k,o2) T2(o2,o3,o1,a) h(o1,c) 1.00000000) D2(i,o1,k,o2) T2(o1,o2,o3,c) h(o3,a)
    3 : (
    4: (
             2.00000000) D3(i,o3,k,o2,o4,o1) T2(o1,o3,o4,a) V2(c1,c1,o2,c)
             2.00000000) D3(i,o3,k,o2,o4,o1) T2(o1,o2,o4,c) V2(c1,c1,o3,a) 2.00000000) D2(i,o3,k,o2) T2(o2,o3,o1,a) V2(c1,c1,o1,c)
    5 : (
    6 : (
    7: (
            2.00000000) D2(i,o3,k,o2) T2(o3,o2,o1,c) V2(c1,c1,o1,a)
            -1.00000000) D3(i,o3,k,o2,o4,o1) T2(o1,o3,o4,a) V2(c1,o2,c1,c) -1.00000000) D3(i,o3,k,o2,o4,o1) T2(o1,o2,o4,c) V2(c1,o3,c1,a)
    8: (
    9: (
   10: (
            -1.00000000) D2(i,o3,k,o2) T2(o2,o3,o1,a) V2(c1,o1,c1,c)
   11: (
            -1.00000000) D2(i,o3,k,o2) T2(o3,o2,o1,c) V2(c1,o1,c1,a)
   12 : ( 1.00000000) D4(i,o4,k,o3,o5,o1,o6,o2) T2(o2,o4,o6,a) V2(o1,o5,o3,c)
   13: (
             1.00000000) D4(i,o3,k,o4,o1,o5,o2,o6) T2(o5,o4,o1,c) V2(o2,o6,o3,a)
             1.00000000) D3(i,o4,k,o3,o5,o2) T2(o2,o4,o1,a) V2(o1,o5,o3,c)
   15 : (
             1.00000000) D3(i,o4,k,o3,o5,o2) T2(o2,o3,o1,c) V2(o1,o5,o4,a)
   16 : (
             1.00000000) D3(i,o4,k,o3,o5,o2) T2(o3,o4,o1,a) V2(o1,c,o2,o5)
            1.00000000) D3(i,o4,k,o3,o5,o2) T2(o4,o3,o1,c) V2(o1,a,o2,o5) 1.00000000) D3(i,o2,k,o3,o1,o4) T2(o4,o3,o1,v1) V2(o2,a,c,v1) 1.00000000) D3(i,o2,k,o3,o1,o4) T2(o4,o2,o1,v1) V2(o3,c,a,v1)
  18 : (
19 : (
  20 : ( 1.00000000) D2(i,o1,k,o2) T2(o1,o2,o3,v1) V2(o3,a,c,v1)
   21: ( 1.00000000) D2(i,o1,k,o2) T2(o2,o1,o3,v1) V2(o3,c,a,v1)
Setting up parameters as default ....
       :+: :+: :+: :+: :+: :+: :+:
    +:+
               +:+
                           +:+ +:+:+ +:+ +:+ +:+
                                                          +:+
    :#::+::# +#++:++# +#+ +:+ +#+ +#+
                                                   +#+ +:+
  +#+
             +#+ +#+
                                +#+ +#+ +#+ +#+
                                                        #+#
 #+#
             #+#
                         #+#
                                  #+# #+#
                                                 #+#
 ###
                                  ### ###
                                                 ########
! * 8 terms are replaced in the linking process ....
The linked formulas ....
0 : (1.00000000) D3(i,o3,k,o2,o4,o1) T2(o1,o3,o4,a) h(o2,c)
        1.00000000) D3(i,o2,k,o3,o1,o4) T2(o4,o3,o1,c) h(o2,a)
1: (
2 : ( 1.00000000) D2(i,o3,k,o2) T2(o2,o3,o1,a) h(o1,c)
3: (1.00000000) D2(i,o1,k,o2) T2(o1,o2,o3,c) h(o3,a)
4 : ( 2.00000000) D3(i,o3,k,o2,o4,o1) T2(o1,o3,o4,a) Y0(o2,c)
5 : (
         2.00000000) D3(i,o3,k,o2,o4,o1) T2(o1,o2,o4,c) Y1(o3,a)
        2.00000000) D2(i,o3,k,o2) T2(o2,o3,o1,a) Y2(o1,c) 2.00000000) D2(i,o3,k,o2) T2(o3,o2,o1,c) Y3(o1,a)
6 : (
7 : (
       -1.00000000) D3(i,o3,k,o2,o4,o1) T2(o1,o3,o4,a) Y4(o2,c)
9: (-1.00000000) D3(i,o3,k,o2,o4,o1) T2(o1,o2,o4,c) Y5(o3,a)
10 : (-1.00000000) D2(i,o3,k,o2) T2(o2,o3,o1,a) Y6(o1,c)
```

```
eclipse sort.dat
  9 11, 12 16:46
                                                                     Page 64/145
11: (
         -1.00000000) D2(i,o3,k,o2) T2(o3,o2,o1,c) Y7(o1,a)
12 : (
         1.00000000) D4(i,o4,k,o3,o5,o1,o6,o2) T2(o2,o4,o6,a) V2(o1,o5,o3,c)
13 : (
          1.00000000) D4(i,o3,k,o4,o1,o5,o2,o6) T2(o5,o4,o1,c) V2(o2,o6,o3,a)
14: (
          1.00000000) D3(i,o4,k,o3,o5,o2) T2(o2,o4,o1,a) V2(o1,o5,o3,c)
        1.00000000) D3(i,o4,k,o3,o5,o2) T2(o2,o3,o1,c) V2(o1,o5,o4,a)
15 : (
        1.00000000) D3(i,o4,k,o3,o5,o2) T2(o3,o4,o1,a) V2(o1,c,o2,o5) 1.00000000) D3(i,o4,k,o3,o5,o2) T2(o4,o3,o1,c) V2(o1,a,o2,o5)
16: (
17 : (
         1.00000000) D3(i,o2,k,o3,o1,o4) T2(o4,o3,o1,v1) V2(o2,a,c,v1)
18 : (
19: (
          1.00000000) D3(i,o2,k,o3,o1,o4) T2(o4,o2,o1,v1) V2(o3,c,a,v1)
20 : (
          1.00000000) D2(i,o1,k,o2) T2(o1,o2,o3,v1) V2(o3,a,c,v1)
        1.00000000) D2(i,o1,k,o2) T2(o2,o1,o3,v1) V2(o3,c,a,v1)
21 : (
The content of each effective tensor ....
Y0 <-- ( 1.00000000) V2(c1,c1,o2,c)
Y1 <-- (
Y2 <-- (
            1.00000000) V2(c1,c1,o3,a)
1.00000000) V2(c1,c1,o1,c)
Y3 <-- (
            1.00000000) V2(c1,c1,o1,a)
            1.00000000) V2(c1,o2,c1,c)
Y4 <-- (
Y5 <-- (
           1.00000000) V2(c1,o3,c1,a)
Y6 <-- ( 1.00000000) V2(c1,o1,c1,c)
Y7 <-- ( 1.00000000) V2(c1,o1,c1,a)
! No.0
! S2(i,k,a,c) <--
! ( 1.00000000) D3(i,o3,k,o2,o4,o1) T2(o1,o3,o4,a) h(o2,c)
o4,a)
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^3)
Case 1 ..... X(i, 03, k, 04, 01, c) <---- ( 1.00000000) D3(i, 03, k, 02, 04, 01) h(o
! Polynomial order is O(o^5v^2)
! Maximum memory usage is O(o^5)
Case 2 ..... X(o1,o3,o4,o2,a,c) <---- ( 1.00000000) T2(o1,o3,o4,a) h(o2,c)
! Polynomial order is O(o^6v^2)
! Maximum memory usage is O(o^4)
! The optimal choice is .....
1: X(i,k,o2,a) <-- ( 1.00000000) D3(i,o3,k,o2,o4,o1) T2(o1,o3,o4,a) 
2: S2(i,k,a,c) <-- ( 1.00000000) X(i,k,o2,a) h(o2,c)
! Scaling
              : O(o^6v^1)
! Max size of X : o^3
! * Begin scaling analysis .... *
for a in {vir}:
  Read T2 from GA for a
  Declare X as a o^3 tensor
  X(a)(i,k,o2) += 1.0 sum(o3,o4,o1) D3(i,o3,k,o2,o4,o1) * T2(o1,o3,o4,)
  for c in {vir}:
   Read S2 from GA for c
    S2_{(c)}(i,k,a) += 1.0 sum(o2) X_{(a)}(i,k,o2,) * h(o2,c)
    Accumulate S2_(c)(i,k,a) for c
! No.1
! S2(i,k,a,c) <--
! ( 1.00000000) D3(i,o2,k,o3,o1,o4) T2(o4,o3,o1,c) h(o2,a)
! Indices of BareAmp are rotated to match with LHS.
Case 0 ..... X(i,o_2,k,c) < ---- (1.00000000) D3(i,o2,k,o3,o1,o4) T2(o4,o3,
o1,c)
```

```
eclipse sort.dat
 9 11, 12 16:46
                                                                       Page 65/145
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^3)
Case 1 ..... X(i,k,o3,o1,o4,a) < ---- (1.00000000) D3(i,o2,k,o3,o1,o4) h(o
2,a)
! Polynomial order is O(o^5v^2)
! Maximum memory usage is O(o^5v^1)
Case 2 ..... X(04,03,01,02,c,a) < ---- ( 1.00000000) T2(04,03,01,c) h(02,a)
! Polynomial order is O(o^6v^2)
! Maximum memory usage is O(o^4v^1)
! The optimal choice is ....
1: X(i,o2,k,c) < -- ( 1.00000000) D3(i,o2,k,o3,o1,o4) T2(o4,o3,o1,c) 2: S2(i,k,a,c) < -- ( 1.00000000) X(i,o2,k,c) h(o2,a)
              : O(o^6v^1)
! Scaling
! Max size of X : o^3
! * Begin scaling analysis .... *
for c in {vir}:
 Read T2 from GA for c
 Read S2 from GA for c
 Declare X as a o^3 tensor
 X_{(c)}(i,o_2,k) += 1.0 \text{ sum}(o_3,o_1,o_4) D_3(i,o_2,k,o_3,o_1,o_4) * T_2(o_4,o_3,o_1,o_4)
 S2 (c)(i,k,a) += 1.0 sum(o2) X (c)(i,o2,k,) * h(o2,a)
 Accumulate S2 (c)(i,k,a) for c
! No.2
! S2(i,k,a,c) <--
! ( 1.00000000) D2(i,o3,k,o2) T2(o2,o3,o1,a) h(o1,c)
Case 0 ..... X(i,k,o1,a) < ---- (1.00000000) D2(i,o3,k,o2) T2(o2,o3,o1,a)
! Polynomial order is O(o^5v^1)
! Maximum memory usage is O(o^3)
Case 1 .... X(\hat{1},03,\hat{k},02,01,c) <---- ( 1.00000000) D2(i,03,k,02) h(01,c)
! Polynomial order is O(o^5v^2)
! Maximum memory usage is O(o^5)
Case 2 ..... X(02,03,a,c) < ---- ( 1.00000000) T2(02,03,01,a) h(01,c)
! Polynomial order is O(o^4v^2)
! Maximum memory usage is O(o^2)
Factorize: Conflict between choices of optimal memory usage and polynomial order
! The optimal choice is .....
1: X(i,k,o1,a) <-- ( 1.00000000) D2(i,o3,k,o2) T2(o2,o3,o1,a)
2: S2(i,k,a,c) <-- ( 1.00000000) X(i,k,o1,a) h(o1,c)
! Scaling
              : O(o^5v^1)
! Max size of X : o^3
! * Begin scaling analysis .... *
for a in {vir}:
 Read T2 from GA for a
 Declare X as a o^3 tensor
 X_{-}(a)(i,k,o1) += 1.0 sum(o3,o2) D2(i,o3,k,o2) * T2(o2,o3,o1,)
 for c in {vir}:
    Read S2 from GA for c
    S2_{(c)}(i,k,a) += 1.0 sum(o1) X_{(a)}(i,k,o1,) * h(o1,c)
    Accumulate S2_(c)(i,k,a) for c
```

```
eclipse sort.dat
  9 11, 12 16:46
                                                                       Page 66/145
! No.3
! S2(i,k,a,c) <--
! ( 1.00000000) D2(i,o1,k,o2) T2(o1,o2,o3,c) h(o3,a)
! Indices of BareAmp are rotated to match with LHS.
Case 0 ..... X(i,k,o3,c) <---- ( 1.00000000) D2(i,o1,k,o2) T2(o1,o2,o3,c)
! Polynomial order is O(o^5v^1)
! Maximum memory usage is O(o^3)
Case 1 ..... X(i,o1,k,o2,o3,a) < ---- ( 1.00000000) D2(i,o1,k,o2) h(o3,a)
! Polynomial order is O(o^5v^2)
! Maximum memory usage is O(o^5v^1)
Case 2 ..... X(o1,o2,c,a) <---- ( 1.00000000) T2(o1,o2,o3,c) h(o3,a)
! Polynomial order is O(o^4v^2)
! Maximum memory usage is O(o^2v^1)
! The optimal choice is .....
1: X(i,k,03,c) \leftarrow (1.00000000) D2(i,01,k,02) T2(01,02,03,c) 2: S2(i,k,a,c) \leftarrow (1.00000000) X(i,k,03,c) h(03,a)
! Scaling
              : O(o^5v^1)
! Max size of X : o^3
! * Begin scaling analysis .... *
for c in {vir}:
  Read T2 from GA for c
  Read S2 from GA for c
  Declare X as a o^3 tensor
  X_{(c)(i,k,o3)} += 1.0 \text{ sum}(o1,o2) D2(i,o1,k,o2) * T2(o1,o2,o3,)
  S2 (c)(i,k,a) += 1.0 sum(o3) X (c)(i,k,o3,) * h(o3,a)
  Accumulate S2_(c)(i,k,a) for c
! No. 4
! S2(i,k,a,c) <--
! ( 2.00000000) D3(i,o3,k,o2,o4,o1) T2(o1,o3,o4,a) Y0(o2,c)
Case 0 ..... X(i,k,o2,a) <---- ( 1.00000000) D3(i,o3,k,o2,o4,o1) T2(o1,o3,
o4,a)
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^3)
Case 1 .... X(i, 0.3, k, 0.4, 0.1, c) < ---- (1.00000000) D3(i, 0.3, k, 0.2, 0.4, 0.1) Y0(
o2,c)
! Polynomial order is O(o^5v^2)
! Maximum memory usage is O(o^5)
Case 2 .... X(01,03,04,02,a,c) <---- ( 1.00000000) T2(01,03,04,a) Y0(02,c
! Polynomial order is O(o^6v^2)
! Maximum memory usage is O(o^4)
! The optimal choice is .....
1: X(i,k,02,a) <-- ( 1.00000000) D3(i,03,k,02,04,01) T2(o1,03,04,a)
2: S2(i,k,a,c) <-- ( 2.00000000) X(i,k,02,a) Y0(o2,c)
! Scaling
              : O(o^6v^1)
! Max size of X : o^3
! * Begin scaling analysis .... *
Declare Y0 as a tensor
for c1 in {core}:
 Read V2 from GA for c1
```

```
eclipse sort.dat
 9 11, 12 16:46
                                                                  Page 67/145
for a in {vir}:
 Read T2 from GA for a
 Declare X as a o^3 tensor
 X_{(a)}(i,k,o2) += 1.0 sum(o3,o4,o1) D3(i,o3,k,o2,o4,o1) * T2(o1,o3,o4,)
 for c in {vir}:
   Read S2 from GA for c
    S2_(c)(i,k,a) += 2 sum(o2) X_(a)(i,k,o2,) * Y0(o2,c)
   Accumulate S2 (c)(i,k,a) for c
! S2(i,k,a,c) <--
! (2.00000000) D3(i,o3,k,o2,o4,o1) T2(o1,o2,o4,c) Y1(o3,a)
! Indices of BareAmp are rotated to match with LHS.
o4,c)
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^3)
Case 1 ..... X(i,k,o2,o4,o1,a) <---- ( 1.00000000) D3(i,o3,k,o2,o4,o1) Y1(
o3,a)
! Polynomial order is O(o^5v^2)
! Maximum memory usage is O(o^5v^1)
Case 2 ..... X(01,02,04,03,c,a) <---- ( 1.00000000) T2(01,02,04,c) Y1(03,a
! Polynomial order is O(o^6v^2)
! Maximum memory usage is O(o^4v^1)
! The optimal choice is .....
1: X(i,03,k,c) < -- ( 1.00000000) D3(i,03,k,02,04,01) T2(01,02,04,c) 2: S2(i,k,a,c) < -- ( 2.00000000) X(i,03,k,c) Y1(03,a)
! Scaling
             : O(o^6v^1)
! Max size of X : o^3
! * Begin scaling analysis .... *
Declare Y1 as a tensor
for c1 in {core}:
 Read V2 from GA for cl
for c in {vir}:
 Read T2 from GA for c
 Read S2 from GA for c
 Declare X as a o^3 tensor
 X_{(c)}(i,03,k) += 1.0 sum(02,04,01) D3(i,03,k,02,04,01) * T2(01,02,04,)
 S2_{(c)}(i,k,a) += 2 sum(o3) X_{(c)}(i,o3,k,) * Y1(o3,a)
 Accumulate S2 (c)(i,k,a) for c
! No.6
! S2(i,k,a,c) <--
! ( 2.00000000) D2(i,o3,k,o2) T2(o2,o3,o1,a) Y2(o1,c)
Case 0 ..... X(i,k,o1,a) <---- ( 1.00000000) D2(i,o3,k,o2) T2(o2,o3,o1,a)
! Polynomial order is O(o^5v^1)
! Maximum memory usage is O(o^3)
Case 1 ..... X(\bar{1}, 03, \bar{k}, 02, 01, c) <---- ( 1.00000000) D2(i, 03, k, 02) Y2(01, c)
! Polynomial order is O(o^5v^2)
! Maximum memory usage is O(o^5)
```

```
eclipse sort.dat
  9 11, 12 16:46
                                                                      Page 68/145
Case 2 ..... X(o2,o3,a,c) <---- (
                                        1.00000000) T2(o2,o3,o1,a) Y2(o1,c)
! Polynomial order is O(o^4v^2)
! Maximum memory usage is O(o^2)
Factorize: Conflict between choices of optimal memory usage and polynomial order
! The optimal choice is .....
1: X(i,k,01,a) <-- ( 1.00000000) D2(i,03,k,02) T2(02,03,01,a)
2: S2(i,k,a,c) <-- ( 2.00000000) X(i,k,01,a) Y2(01,c)
! Scaling : O(o^5v^1)
! Max size of X : o^3
! * Begin scaling analysis .... *
Declare Y2 as a tensor
for cl in {core}:
 Read V2 from GA for c1
for a in {vir}:
 Read T2 from GA for a
  Declare X as a o^3 tensor
  X_{(a)(i,k,o1)} += 1.0 \text{ sum}(o3,o2) D2(i,o3,k,o2) * T2(o2,o3,o1,)
  for c in {vir}:
    Read S2 from GA for c
    S2_{(c)(i,k,a)} += 2 sum(o1) X_{(a)(i,k,o1,)} * Y2(o1,c)
    Accumulate S2 (c)(i,k,a) for c
! No.7
! S2(i,k,a,c) <--
! ( 2.00000000) D2(i,o3,k,o2) T2(o3,o2,o1,c) Y3(o1,a)
! Indices of BareAmp are rotated to match with LHS.
Case 0 ..... X(i,k,o1,c) <---- ( 1.00000000) D2(i,o3,k,o2) T2(o3,o2,o1,c)
! Polynomial order is O(o^5v^1)
! Maximum memory usage is O(o^3)
Case 1 ..... X(\bar{1}, 03, \bar{k}, 02, 01, a) < ---- ( 1.00000000) D2(i, 03, k, 02) Y3(01, a)
! Polynomial order is O(o^5v^2)
! Maximum memory usage is O(o^5v^1)
Case 2 ..... X(03,02,c,a) <---- ( 1.00000000) T2(03,02,01,c) Y3(01,a)
! Polynomial order is O(o^4v^2)
! Maximum memory usage is O(o^2v^1)
! The optimal choice is .....
1: X(i,k,o1,c) <-- ( 1.00000000) D2(i,o3,k,o2) T2(o3,o2,o1,c)
2: S2(i,k,a,c) < -- ( 2.00000000) X(i,k,o1,c) Y3(o1,a)
! Scaling
              : O(o^5v^1)
! Max size of X : o^3
! * Begin scaling analysis .... *
Declare Y3 as a tensor
for c1 in {core}:
 Read V2 from GA for cl
for c in {vir}:
  Read T2 from GA for c
  Read S2 from GA for c
  Declare X as a o^3 tensor
  X_{(c)}(i,k,o1) += 1.0 \text{ sum}(o3,o2) D2(i,o3,k,o2) * T2(o3,o2,o1,)
  S2_{(c)}(i,k,a) += 2 sum(o1) X_{(c)}(i,k,o1,) * Y3(o1,a)
```

```
eclipse sort.dat
 9 11, 12 16:46
                                                                 Page 69/145
 Accumulate S2 (c)(i,k,a) for c
! No.8
! S2(i,k,a,c) <--
! ( -1.00000000) D3(i,o3,k,o2,o4,o1) T2(o1,o3,o4,a) Y4(o2,c)
o4,a)
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^3)
Case 1 ..... X(i,o3,k,o4,o1,c) < ---- (1.00000000) D3(i,o3,k,o2,o4,o1) Y4(
o2,c)
! Polynomial order is O(o^5v^2)
! Maximum memory usage is O(o^5)
Case 2 ..... X(o1,o3,o4,o2,a,c) <---- ( 1.00000000) T2(o1,o3,o4,a) Y4(o2,c
! Polynomial order is O(o^6v^2)
! Maximum memory usage is O(o^4)
! The optimal choice is ....
1: X(i,k,02,a) < -- ( 1.00000000) D3(i,03,k,02,04,01) T2(01,03,04,a) 2: S2(i,k,a,c) < -- ( -1.00000000) X(i,k,02,a) Y4(02,c)
! Scaling : O(o^6v^1)
! Max size of X : o^3
! * Begin scaling analysis .... *
Declare Y4 as a tensor
for c1 in {core}:
 Read V2 from GA for c1
for a in {vir}:
 Read T2 from GA for a
 Declare X as a o^3 tensor
 X_{(a)}(i,k,o2) += 1.0 sum(o3,o4,o1) D3(i,o3,k,o2,o4,o1) * T2(o1,o3,o4,)
 for c in {vir}:
   Read S2 from GA for c
   S2_{(c)}(i,k,a) += -1 sum(o2) X_{(a)}(i,k,o2,) * Y4(o2,c)
   Accumulate S2_(c)(i,k,a) for c
1 No. 9
! S2(i,k,a,c) <--
! (-1.00000000) D3(i,o3,k,o2,o4,o1) T2(o1,o2,o4,c) Y5(o3,a)
! Indices of BareAmp are rotated to match with LHS.
Case 0 \ldots X(i,o3,k,c) < ---- (1.00000000) D3(i,o3,k,o2.o4.o1) T2(o1.o2.
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^3)
Case 1 ..... X(i,k,o2,o4,o1,a) <---- ( 1.00000000) D3(i,o3,k,o2,o4,o1) Y5(
! Polynomial order is O(o^5v^2)
! Maximum memory usage is O(o^5v^1)
Case 2 ..... X(01,02,04,03,c,a) <---- ( 1.00000000) T2(01,02,04,c) Y5(03,a
! Polynomial order is O(o^6v^2)
! Maximum memory usage is O(o^4v^1)
! The optimal choice is .....
1: X(i,03,k,c) < -- (1.00000000) D3(i,03,k,02,04,01) T2(01,02,04,c)
```

```
eclipse sort.dat
                                                                      Page 70/145
  9 11, 12 16:46
2: S2(i,k,a,c) <-- ( -1.00000000) X(i,o3,k,c) Y5(o3,a)
! Scaling
              : O(o^6v^1)
! Max size of X : o^3
! * Begin scaling analysis .... *
Declare Y5 as a tensor
for c1 in {core}:
  Read V2 from GA for c1
for c in {vir}:
  Read T2 from GA for c
  Read S2 from GA for c
  Declare X as a o^3 tensor
  X(c)(i,03,k) += 1.0 sum(02,04,01) D3(i,03,k,02,04,01) * T2(01,02,04,)
  S2 (c)(i,k,a) += -1 sum(o3) X (c)(i,o3,k,) * Y5(o3,a)
  Accumulate S2 (c)(i,k,a) for c
! No.10
! S2(i,k,a,c) <--
! (-1.00000000) D2(i,o3,k,o2) T2(o2,o3,o1,a) Y6(o1,c)
Case 0 ..... X(i,k,o1,a) <---- ( 1.00000000) D2(i,o3,k,o2) T2(o2,o3,o1,a)
! Polynomial order is O(o^5v^1)
! Maximum memory usage is O(o^3)
Case 1 ..... X(i,03,k,02,01,c) < ---- (1.00000000) D2(i,03,k,02) Y6(01,c)
! Polynomial order is O(o^5v^2)
! Maximum memory usage is O(o^5)
Case 2 ..... X(02,03,a,c) < ---- (1.00000000) T2(02,03,01,a) Y6(01,c)
! Polynomial order is O(o^4v^2)
! Maximum memory usage is O(o^2)
Factorize: Conflict between choices of optimal memory usage and polynomial order
! The optimal choice is .....
1: X(i,k,ol,a) <-- ( 1.00000000) D2(i,o3,k,o2) T2(o2,o3,ol,a) 
2: S2(i,k,a,c) <-- ( -1.00000000) X(i,k,ol,a) Y6(ol,c)
! Scaling
              : O(o^5v^1)
! Max size of X : o^3
! * Begin scaling analysis .... *
Declare Y6 as a tensor
for c1 in {core}:
  Read V2 from GA for cl
for a in {vir}:
 Read T2 from GA for a
  Declare X as a o^3 tensor
  X_{(a)}(i,k,o1) += 1.0 \text{ sum}(o3,o2) D2(i,o3,k,o2) * T2(o2,o3,o1,)
  for c in {vir}:
   Read S2 from GA for c
    S2_{(c)}(i,k,a) += -1 sum(o1) X_{(a)}(i,k,o1,) * Y6(o1,c)
   Accumulate S2_(c)(i,k,a) for c
! No.11
```

```
eclipse sort.dat
 9 11, 12 16:46
                                                                 Page 71/145
! S2(i,k,a,c) <--
! ( -1.00000000) D2(i,o3,k,o2) T2(o3,o2,o1,c) Y7(o1,a)
! Indices of BareAmp are rotated to match with LHS.
Case 0 ..... X(i,k,o1,c) < ---- (1.00000000) D2(i,o3,k,o2) T2(o3,o2,o1,c)
! Polynomial order is O(o^5v^1)
! Maximum memory usage is O(o^3)
Case 1 ..... X(i,o3,k,o2,o1,a) < ---- (1.00000000) D2(i,o3,k,o2) Y7(o1,a)
! Polynomial order is O(o^5v^2)
! Maximum memory usage is O(o^5v^1)
Case 2 ..... X(03,02,c,a) <---- ( 1.00000000) T2(03,02,01,c) Y7(01,a)
! Polynomial order is O(o^4v^2)
! Maximum memory usage is O(o^2v^1)
! The optimal choice is .....
1: X(i,k,o1,c) <-- ( 1.00000000) D2(i,o3,k,o2) T2(o3,o2,o1,c)
2: S2(i,k,a,c) < -- (-1.00000000) X(i,k,o1,c) Y7(o1,a)
! Scaling
             : O(o^5v^1)
! Max size of X : o^3
! * Begin scaling analysis .... *
Declare Y7 as a tensor
for c1 in {core}:
 Read V2 from GA for c1
for c in {vir}:
 Read T2 from GA for c
 Read S2 from GA for c
 Declare X as a o^3 tensor
 X(c)(i,k,o1) += 1.0 sum(o3,o2) D2(i,o3,k,o2) * T2(o3,o2,o1,)
 S2_(c)(i,k,a) += -1 sum(o1) X_(c)(i,k,o1,) * Y7(o1,a)
 Accumulate S2 (c)(i,k,a) for c
! No.12
! S2(i,k,a,c) <--
! ( 1.00000000) D4(i,o4,k,o3,o5,o1,o6,o2) T2(o2,o4,o6,a) V2(o1,o5,o3,c)
! Indices of ERI are rotated to match with LHS.
! *** D4(i,04,k,03,05,01,06,02) T2(02,04,06,a) is skipped due to the priority
Case 1 .... X(i,o4,k,o6,o2,c) <---- ( 1.00000000) D4(i,o4,k,o3,o5,o1,o6,o
2) V2(c,o3,o1,o5)
! Polynomial order is O(o^8v^1)
! Maximum memory usage is O(o^3)
Case 2 ..... X(o2,o4,o6,o3,o1,o5,a,c) <---- ( 1.00000000) T2(o2,o4,o6,a) V
2(c,o3,o1,o5)
! Polynomial order is O(o^8v^2)
! Maximum memory usage is O(o^5)
! The optimal choice is .....
1: X(i,04,k,06,02,c) < -- ( 1.00000000) D4(i,04,k,03,05,01,06,02) V2(c,03,0)
1,05)
2: S2(i,k,a,c) <-- ( 1.00000000) T2(o2,o4,o6,a) X(i,o4,k,o6,o2,c)
! Scaling : 0(o^8v^1)
! Max size of X : o^3
! * Begin scaling analysis .... *
for c in {vir}:
 Read V2 from GA for c
 Read S2 from GA for c
 for i in {occ}:
   for o4 in {occ}:
```

```
eclipse sort.dat
  9 11, 12 16:46
                                                                    Page 72/145
      Read D4 from GA for i, o4
      Declare X as a o^3 tensor
      X_{(c,i,o4)}(k,o6,o2) += 1.0 sum(o3,o1,o5) V2(,o3,o1,o5) * D4(,,k,o3,o5,o1,o5)
6,02)
      for a in {vir}
        Read T2 from GA for a
        S2_{(c)}(i,k,a) += 1.0 sum(02,06) T2(02,04,06,) * X_{(c,i,04)}(,,k,06,02,)
        Accumulate S2 (c)(i,k,a) for c
 ! No.13
! S2(i,k,a,c) <--
! ( 1.00000000) D4(i,o3,k,o4,o1,o5,o2,o6) T2(o5,o4,o1,c) V2(o2,o6,o3,a)
! Indices of BareAmp are rotated to match with LHS.
! Indices of ERI and D4 are rotated to match with each other.
 *TEST* ( 1.00000000) D4(o2,o6,i,o3,k,o4,o1,o5) T2(o5,o4,o1,c) V2(o2,o6,o3,a)
 ! *** D4(02,06,i,03,k,04,01,05) T2(05,04,01,c) is skipped due to the priority
Case 1 .... X(i,k,04,01,05,a) < ---- (1.00000000) D4(02,06,i,03,k,04,01,0)
5) V2(o2,o6,o3,a)
 ! Polynomial order is O(o^8v^1)
 ! Maximum memory usage is O(o^5v^1)
 Case 2 ..... X(05,04,01,02,06,03,c,a) <---- ( 1.00000000) T2(05,04,01,c) V
2(o2,o6,o3,a)
! Polynomial order is O(o^8v^2)
! Maximum memory usage is O(o^4v^1)
! Case 0 is skipped due to the priority of ERI ....
 ! The optimal choice is .....
1: X(05,04,01,02,06,03,c,a) < -- ( 1.00000000) T2(05,04,01,c) V2(02,06,03,a)
2: S2(i,k,a,c) < -- ( 1.00000000) D4(o2,o6,i,o3,k,o4,o1,o5) X(o5,o4,o1,o2,o6)
 ,o3,c,a)
 ! Scaling
              : O(o^8v^2)
 ! Max size of X : o^4v^1
 ! * Begin scaling analysis .... *
 for o2 in {occ}:
  Read V2 from GA for o2
  for o6 in {occ}:
    Read D4 from GA for o2, o6
    for c in {vir}:
      Read T2 from GA for c
      Read S2 from GA for c
      Declare X as a o^4v^1 tensor
      X_{(02,06,c)(05,04,01,03,a)} += 1.0 \text{ sum}() V2(,06,03,a) * T2(05,04,01,)
      S2_{(c)}(i,k,a) += 1.0 \text{ sum}(03,04,01,05) D4(,,i,03,k,04,01,05) * X_{(02,06,c)}(
o5,o4,o1,,,o3,,a)
      Accumulate S2_(c)(i,k,a) for c
! No.14
! S2(i,k,a,c) <--
! ( 1.00000000) D3(i,o4,k,o3,o5,o2) T2(o2,o4,o1,a) V2(o1,o5,o3,c)
! Indices of ERI are rotated to match with LHS.
! *** D3(i,o4,k,o3,o5,o2) T2(o2,o4,o1,a) is skipped due to the priority
Case 1 ..... X(i,o4,k,o2,o1,c) <---- ( 1.00000000) D3(i,o4,k,o3,o5,o2) V2(
```

```
eclipse sort.dat
 9 11, 12 16:46
                                                                    Page 73/145
c, o3, o1, o5)
! Polynomial order is O(o^7v^1)
! Maximum memory usage is O(o^5)
Case 2 ..... X(02,04,03,05,a,c) < ---- ( 1.00000000) T2(02,04,01,a) V2(c,03)
,01,05)
! Polynomial order is O(o^6v^2)
! Maximum memory usage is O(o^4)
Factorize: Conflict between choices of optimal memory usage and polynomial order
! The optimal choice is .....
1: X(i,o4,k,o2,o1,c) <-- ( 1.00000000) D3(i,o4,k,o3,o5,o2) V2(c,o3,o1,o5)
2: S2(i,k,a,c) <-- ( 1.00000000) T2(o2,o4,o1,a) X(i,o4,k,o2,o1,c)
! Scaling
              : O(o^7v^1)
! Max size of X : o^5
! * Begin scaling analysis .... *
for c in {vir}:
 Read V2 from GA for c
 Read S2 from GA for c
 Declare X as a o^5 tensor
 X(c)(i,04,k,02,01) += 1.0 \text{ sum}(03,05) V2(,03,01,05) * D3(i,04,k,03,05,02)
 for a in {vir}
   Read T2 from GA for a
   S2(c)(i,k,a) += 1.0 sum(o2,o4,o1) T2(o2,o4,o1,) * X(c)(i,o4,k,o2,o1,)
   Accumulate S2 (c)(i,k,a) for c
! No.15
! S2(i,k,a,c) <--
! (1.00000000) D3(i,04,k,03,05,02) T2(02,03,01,c) V2(01,05,04,a)
! Indices of BareAmp are rotated to match with LHS.
! The indices of ERI are rotated to became virtual.
! *** D3(i,o4,k,o3,o5,o2) T2(o2,o3,o1,c) is skipped due to the priority
Case 1 .... X(i,k,o3,o2,o1,a) < ---- (1.00000000) D3(i,o4,k,o3,o5,o2) V2(
a,o4,o1,o5)
! Polynomial order is O(o^7v^1)
! Maximum memory usage is O(o^5)
Case 2 ..... X(02.03.04.05.c.a) < ---- ( 1.00000000) T2(02.03.01.c) V2(a.04.05.c.a) < ---- ( 1.00000000) T2(02.03.01.c.a) V2(a.04.05.c.a)
,01,05)
! Polynomial order is O(o^6v^2)
! Maximum memory usage is O(o^4)
Factorize: Conflict between choices of optimal memory usage and polynomial order
! The optimal choice is .....
1: X(i,k,03,02,01,a) < -- (1.00000000) D3(i,04,k,03,05,02) V2(a,04,01,05)
2: S2(i,k,a,c) <-- ( 1.00000000) T2(o2,o3,o1,c) X(i,k,o3,o2,o1,a)
! Scaling
            : O(o^7v^1)
! Max size of X : o^5
! * Begin scaling analysis .... *
for a in {vir}:
 Read V2 from GA for a
 Declare X as a o^5 tensor
 X_{(a)}(i,k,o3,o2,o1) += 1.0 sum(o4,o5) V2(,o4,o1,o5) * D3(i,o4,k,o3,o5,o2)
 for c in {vir}:
   Read S2 from GA for c
   Read T2 from GA for c
```

```
eclipse sort.dat
  9 11, 12 16:46
                                                                   Page 74/145
    S2_{(c)(i,k,a)} += 1.0 sum(o2,o3,o1) T2(o2,o3,o1,) * X_{(a)(i,k,o3,o2,o1,)}
   Accumulate S2 (c)(i,k,a) for c
! No.16
! S2(i,k,a,c) <--
! ( 1.00000000) D3(i,o4,k,o3,o5,o2) T2(o3,o4,o1,a) V2(o1,c,o2,o5)
! Indices of ERI are rotated to match with LHS.
! *** D3(i,o4,k,o3,o5,o2) T2(o3,o4,o1,a) is skipped due to the priority
Case 1 ..... X(i, 04, k, 03, 01, c) < ---- ( 1.00000000) D3(i, 04, k, 03, 05, 02) V2(
c,o1,o2,o5)
! Polynomial order is O(o^7v^1)
! Maximum memory usage is O(o^5)
Case 2 ..... X(03,04,02,05,a,c) <---- ( 1.00000000) T2(03,04,01,a) V2(c,01
! Polynomial order is O(o^6v^2)
! Maximum memory usage is O(o^4)
Factorize: Conflict between choices of optimal memory usage and polynomial order
! The optimal choice is .....
1: X(i,o4,k,o3,o1,c) <-- ( 1.00000000) D3(i,o4,k,o3,o5,o2) V2(c,o1,o2,o5)
2: S2(i,k,a,c) < -- (1.00000000) T2(03,04,01,a) X(i,04,k,03,01,c)
! Scaling
             : O(o^7v^1)
! Max size of X : o^5
! * Begin scaling analysis .... *
for c in {vir}:
 Read V2 from GA for c
  Read S2 from GA for c
  Declare X as a o^5 tensor
  X(c)(i,04,k,03,01) += 1.0 sum(02,05) V2(,01,02,05) * D3(i,04,k,03,05,02)
  for a in {vir}
   Read T2 from GA for a
    S2_{(c)}(i,k,a) += 1.0 \text{ sum}(03,04,01) T2(03,04,01,) * X_{(c)}(i,04,k,03,01,)
   Accumulate S2_(c)(i,k,a) for c
! No.17
! S2(i,k,a,c) <--
! ( 1.00000000) D3(i,o4,k,o3,o5,o2) T2(o4,o3,o1,c) V2(o1,a,o2,o5)
! Indices of BareAmp are rotated to match with LHS.
! The indices of ERI are rotated to became virtual.
! *** D3(i,o4,k,o3,o5,o2) T2(o4,o3,o1,c) is skipped due to the priority
Case 1 ..... X(i,o4,k,o3,o1,a) <---- ( 1.00000000) D3(i,o4,k,o3,o5,o2) V2(
a, o1, o2, o5)
! Polynomial order is O(o^7v^1)
! Maximum memory usage is O(o^5)
Case 2 ..... X(04,03,02,05,c,a) < ---- ( 1.00000000) T2(04,03,01,c) V2(a,01)
,02,05)
! Polynomial order is O(o^6v^2)
! Maximum memory usage is O(o^4)
Factorize: Conflict between choices of optimal memory usage and polynomial order
! The optimal choice is .....
1: X(i,04,k,03,01,a) < -- (1.00000000) D3(i,04,k,03,05,02) V2(a,01,02,05)
2: S2(i,k,a,c) < -- ( 1.00000000) T2(04,03,01,c) X(i,04,k,03,01,a)
```

```
eclipse_sort.dat
                                                                   Page 75/145
 9 11, 12 16:46
             : O(o^7v^1)
! Scaling
! Max size of X : o^5
! * Begin scaling analysis .... *
for a in {vir}:
 Read V2 from GA for a
 Declare X as a o^5 tensor
 X (a)(i,04,k,03,01) += 1.0 sum(02,05) V2(,01,02,05) * D3(i,04,k,03,05,02)
 for c in {vir}:
    Read S2 from GA for c
    Read T2 from GA for c
   S2_{(c)}(i,k,a) += 1.0 sum(04,03,01) T2(04,03,01,) * X_{(a)}(i,04,k,03,01,)
    Accumulate S2 (c)(i,k,a) for c
! No.18
! S2(i,k,a,c) <--
! ( 1.00000000) D3(i,o2,k,o3,o1,o4) T2(o4,o3,o1,v1) V2(o2,a,c,v1)
! Indices of ERI are rotated to match with LHS.
! *** D3(i,o2,k,o3,o1,o4) T2(o4,o3,o1,v1) is skipped due to the priority
Case 1 ..... X(i,k,o3,o1,o4,c,v1,a) < ---- (1.00000000) D3(i,o2,k,o3,o1,o4
) V2(c,v1,o2,a)
! Polynomial order is O(o^6v^3)
! Maximum memory usage is O(o^5v^1)
Case 2 ..... X(o4,o3,o1,o2,c,a) <---- ( 1.00000000) T2(o4,o3,o1,v1) V2(c,v
1,o2,a)
! Polynomial order is O(o^6v^2)
! Maximum memory usage is O(o^4v^1)
! The optimal choice is .....
1: X(04,03,01,02,c,a) < --
                               1.000000000 T2(o4,o3,o1,v1) V2(c,v1,o2,a)
2: S2(i,k,a,c) < -- ( 1.00000000) D3(i,o2,k,o3,o1,o4) \times (o4,o3,o1,o2,c,a)
! Scaling
              : O(o^6v^2)
! Max size of X : o^4v^1
! * Begin scaling analysis .... *
for c in {vir}:
 Read V2 from GA for c
 Read S2 from GA for c
 Declare X as a o^4v^1 tensor
 for v1 in {vir}:
   Read T2 from GA for v1
   X_{(c)}(04,03,01,02,a) += 1.0 sum() V2(,v1,02,a) * T2(04,03,01,)
 S2_{(c)}(i,k,a) += 1.0 \text{ sum}(02,03,01,04) D3(i,02,k,03,01,04) * X_{(c)}(04,03,01,02,01,02)
,a)
 Accumulate S2_(c)(i,k,a) for c
! No.19
! S2(i,k,a,c) <--
     1.00000000) D3(i,o2,k,o3,o1,o4) T2(o4,o2,o1,v1) V2(o3,c,a,v1)
! Indices of ERI are rotated to match with LHS.
! *** D3(i,o2,k,o3,o1,o4) T2(o4,o2,o1,v1) is skipped due to the priority
Case 1 .... X(i,02,k,01,04,c,a,v1) < ---- ( 1.00000000) D3(i,02,k,03,01,04)
) V2(c,o3,a,v1)
```

```
eclipse sort.dat
 9 11, 12 16:46
                                                                 Page 76/145
! Polynomial order is O(o^6v^3)
! Maximum memory usage is O(o^5v^1)
Case 2 ..... X(04,02,01,03,c,a) < ---- ( 1.00000000) T2(04,02,01,v1) V2(c,o)
3,a,v1)
! Polynomial order is O(o^6v^2)
! Maximum memory usage is O(o^4v^1)
! The optimal choice is .....
1: X(o4,o2,o1,o3,c,a) <-- ( 1.00000000) T2(o4,o2,o1,v1) V2(c,o3,a,v1)
2: S2(i,k,a,c) < -- (1.00000000) D3(i,o2,k,o3,o1,o4) X(o4,o2,o1,o3,c,a)
! Scaling
             : O(o^6v^2)
! Max size of X : o^4v^1
! * Begin scaling analysis .... *
for c in {vir}:
 Read V2 from GA for c
  Read S2 from GA for c
  Declare X as a o^4v^1 tensor
  for v1 in {vir}:
   Read T2 from GA for v1
   X_{(c)}(04,02,01,03,a) += 1.0 sum() V2(,03,a,v1) * T2(04,02,01,)
 S2_{(c)}(i,k,a) += 1.0 \text{ sum}(02,03,01,04) D3(i,02,k,03,01,04) * X_{(c)}(04,02,01,03,01,04)
,a)
 Accumulate S2 (c)(i,k,a) for c
! No.20
! S2(i,k,a,c) <--
! ( 1.00000000) D2(i,o1,k,o2) T2(o1,o2,o3,v1) V2(o3,a,c,v1)
! Indices of ERI are rotated to match with LHS.
! *** D2(i,o1,k,o2) T2(o1,o2,o3,v1) is skipped due to the priority
.v1.o3.a)
! Polynomial order is O(o^5v^3)
! Maximum memory usage is O(o^5v^1)
Case 2 ..... X(o1,o2,c,a) <---- ( 1.00000000) T2(o1,o2,o3,v1) V2(c,v1,o3,a
! Polynomial order is O(o^3v^3)
! Maximum memory usage is O(o^2v^1)
! The optimal choice is .....
1: X(01,02,c,a) < -- ( 1.00000000) T2(01,02,03,v1) V2(c,v1,03,a)
2: S2(i,k,a,c) < -- (1.00000000) D2(i,o1,k,o2) X(o1,o2,c,a)
! Scaling
              : O(o^3v^3)
! Max size of X : o^2v^1
! * Begin scaling analysis .... *
for c in {vir}:
 Read V2 from GA for c
  Read S2 from GA for c
  Declare X as a o^2v^1 tensor
  for v1 in {vir}:
   Read T2 from GA for v1
   X_{(c)}(01,02,a) += 1.0 sum(03) V2(,v1,03,a) * T2(01,02,03,)
  S2_{(c)(i,k,a)} += 1.0 sum(o1,o2) D2(i,o1,k,o2) * X_{(c)(o1,o2,a)}
 Accumulate S2_(c)(i,k,a) for c
```

```
eclipse sort.dat
! S2(i,k,a,c) <--
! ( 1.00000000) D2(i,o1,k,o2) T2(o2,o1,o3,v1) V2(o3,c,a,v1)
! Indices of ERI are rotated to match with LHS.
! *** D2(i,o1,k,o2) T2(o2,o1,o3,v1) is skipped due to the priority
Case 1 .... X(i,o1,k,o2,o3,c,a,v1) <---- ( 1.00000000) D2(i,o1,k,o2) V2(c
,o3,a,v1)
! Polynomial order is O(o^5v^3)
! Maximum memory usage is O(o^5v^1)
Case 2 ..... X(o2,o1,c,a) <---- ( 1.00000000) T2(o2,o1,o3,v1) V2(c,o3,a,v1)
! Polynomial order is O(o^3v^3)
! Maximum memory usage is O(o^2v^1)
! The optimal choice is .....
1: X(o2,o1,c,a) <-- ( 1.00000000) T2(o2,o1,o3,v1) V2(c,o3,a,v1)
2: S2(i,k,a,c) <-- (
                       1.000000000) D2(i,o1,k,o2) X(o2,o1,c,a)
! Scaling
            : O(o^3v^3)
! Max size of X : o^2v^1
! * Begin scaling analysis .... *
for c in {vir}:
 Read V2 from GA for c
 Read S2 from GA for c
 Declare X as a o^2v^1 tensor
 for v1 in {vir}:
   Read T2 from GA for v1
   X_{(c)(o2,o1,a)} += 1.0 sum(o3) V2(,o3,a,v1) * T2(o2,o1,o3,)
 S2(c)(i,k,a) += 1.0 sum(o1,o2) D2(i,o1,k,o2) * X(c)(o2,o1,a)
 Accumulate S2 (c)(i,k,a) for c
* 3 <000v/00vv>
    0.50000000) T2(o1,o2,v1,a) V2(c1,o3,c2,v1) E4(c1,i,k,o3,c2,m,o2,o1)
    0.50000000) T2(o1,o2,v1,a) V2(c1,m,c2,v1) E3(c1,i,k,c2,o1,o2)
    0.50000000) T2(01,02,a,v1) V2(c1,03,c2,v1) E4(c1,i,k,03,c2,m,01,02)
    0.50000000) T2(o1,o2,a,v1) V2(c1,m,c2,v1) E3(c1,i,k,c2,o2,o1)
     0.50000000) \ \ T2(o1,o2,v1,a) \ \ V2(c1,c2,v1,o3) \ \ E4(c1,i,k,o3,o1,m,o2,c2) 
    0.50000000) T2(o1,o2,v1,a) V2(c1,c2,v1,m) E3(c1,i,k,o1,c2,o2)
    0.50000000) T2(01,02,a,v1) V2(c1,c2,v1,o3) E4(c1,i,k,o3,o2,m,o1,c2)
    0.50000000) T2(o1,o2,a,v1) V2(c1,c2,v1,m) E3(c1,i,k,o2,c2,o1)
    0.50000000) T2(o1,o2,v1,a) V2(c1,c2,v1,o3) E4(c1,i,k,o3,o1,m,o2,c2)
    0.50000000) T2(o1,o2,v1,a) V2(c1,c2,v1,m) E3(c1,i,k,o1,c2,o2)
    0.50000000) T2(o1,o2,a,v1) V2(c1,c2,v1,o3) E4(c1,i,k,o3,o2,m,o1,c2)
    0.50000000) T2(o1,o2,a,v1) V2(c1,c2,v1,m) E3(c1,i,k,o2,c2,o1)
    0.50000000) T2(o1,o2,v1,a) V2(c1,o3,c2,v1) E4(c1,i,k,o3,c2,m,o2,o1)
    0.50000000) T2(o1,o2,v1,a) V2(c1,m,c2,v1) E3(c1,i,k,c2,o1,o2)
    0.50000000) T2(o1,o2,a,v1) V2(c1,o3,c2,v1) E4(c1,i,k,o3,c2,m,o1,o2)
    0.50000000) T2(o1,o2,a,v1) V2(c1,m,c2,v1) E3(c1,i,k,c2,o2,o1)
    0.50000000) T2(o1,o2,v1,a) V2(o3,o4,o5,v1) E4(i,k,o3,o4,m,o2,o5,o1)
    0.50000000) T2(o1,o2,v1,a) V2(m,o3,o4,v1) E3(i,k,o3,o4,o2,o1)
    0.50000000) T2(o1,o2,v1,a) V2(m,o3,v1,o4) E3(i,k,o3,o1,o2,o4)
     0.50000000) \ T2(o1,o2,a,v1) \ V2(o3,o4,o5,v1) \ E4(i,k,o3,o4,m,o1,o5,o2) \\
    0.50000000) T2(o1,o2,a,v1) V2(m,o3,o4,v1) E3(i,k,o3,o4,o1,o2)
    0.50000000) T2(o1,o2,a,v1) V2(m,o3,v1,o4) E3(i,k,o3,o2,o1,o4)
    0.50000000) T2(01,02,v1,a) V2(03,04,v1,05) E4(i,k,03,04,m,02,01,05)
    0.50000000) T2(o1,o2,v1,a) V2(m,o3,v1,o4) E3(i,k,o3,o1,o2,o4)
    0.50000000) T2(o1,o2,v1,a) V2(m,o3,o4,v1) E3(i,k,o3,o4,o2,o1)
```

```
eclipse sort.dat
        9 11, 12 16:46
                                                                                                                     Page 78/145
             0.50000000) T2(01,02,a,v1) V2(03,04,v1,05) E4(i,k,03,04,m,01,02,05)
             0.50000000) T2(o1,o2,a,v1) V2(m,o3,v1,o4) E3(i,k,o3,o2,o1,o4)
             0.50000000) T2(o1,o2,a,v1) V2(m,o3,o4,v1) E3(i,k,o3,o4,o1,o2)
             0.50000000) T2(01,02,v1,v2) V2(03,a,v1,v2) E3(i,k,03,m,02,01)
             0.50000000) T2(o1,o2,v1,v2) V2(m,a,v1,v2) E2(i,k,o1,o2)
             0.50000000) T2(o1,o2,v1,v2) V2(o3,a,v2,v1) E3(i,k,o3,m,o1,o2)
             0.50000000) T2(o1,o2,v1,v2) V2(m,a,v2,v1) E2(i,k,o2,o1)
             0.50000000) T2(o1,o2,v1,v2) V2(o3,a,v1,v2) E3(i,k,o3,m,o2,o1)
             0.50000000) T2(o1,o2,v1,v2) V2(m,a,v1,v2) E2(i,k,o1,o2) 0.50000000) T2(o1,o2,v1,v2) V2(o3,a,v2,v1) E3(i,k,o3,m,o1,o2)
             0.50000000) T2(o1,o2,v1,v2) V2(m,a,v2,v1) E2(i,k,o2,o1)
     Decompose RDMs .....
     < RESULT >
                          1.00000000) D3(i,k,o3,m,o2,o1) T2(o1,o2,v1,a) h(o3,v1)
           0 : (
           1: (
                          1.00000000) D2(i,k,o2,o1) T2(o2,o1,v1,a) h(m,v1)
                          1.00000000) D3(i,k,o1,m,o2,o3) T2(o2,o3,a,v1) h(o1,v1)
         3 : (
                          1.00000000) D2(i,k,o1,o2) T2(o2,o1,a,v1) h(m,v1)
          4 : (
                           2.00000000) D3(i,k,o3,m,o2,o1) T2(o1,o2,v1,a) V2(c1,o3,c1,v1)
          5 : (
6 : (
                           2.00000000) D2(i,k,o2,o1) T2(o2,o1,v1,a) V2(c1,m,c1,v1)
                          2.00000000) D3(i,k,o3,m,o2,o1) T2(o2,o1,a,v1) V2(c1,o3,c1,v1)
           7 : (
                          2.00000000) D2(i,k,o2,o1) T2(o1,o2,a,v1) V2(c1,m,c1,v1)
            8 : ( -1.00000000) \ D3(i,k,o3,m,o2,o1) \ T2(o1,o2,v1,a) \ V2(c1,c1,o3,v1)
           9: ( -1.00000000) D2(i,k,o2,o1) T2(o2,o1,v1,a) V2(c1,c1,m,v1)
          10 : (
                        -1.00000000) D3(i,k,o3,m,o2,o1) T2(o2,o1,a,v1) V2(c1,c1,o3,v1)
          11: (
                         -1.00000000) D2(i,k,o2,o1) T2(o1,o2,a,v1) V2(c1,c1,m,v1)
          12: (
                         1.00000000) D4(i,k,o5,o4,m,o3,o2,o1) T2(o1,o3,v1,a) V2(o5,o4,o2,v1)
                          1.000000000) D3(i,k,o4,o3,o2,o1) T2(o1,o2,v1,a) V2(m,o4,o3,v1)
          14: (
                           1.00000000) D3(i,k,o4,o3,o2,o1) T2(o3,o2,v1,a) V2(m,o4,v1,o1)
          15 : (
                           1.00000000) D4(i,k,o2,o1,m,o3,o5,o4) T2(o3,o4,a,v1) V2(o2,o1,o5,v1)
                           1.00000000) D3(i,k,o4,o3,o2,o1) T2(o2,o1,a,v1) V2(m,o4,o3,v1)
                          1.00000000) D3(i,k,o4,o3,o2,o1) T2(o2,o3,a,v1) V2(m,o4,v1,o1)
          17 : (
          18: (
                           1.00000000) D3(i,k,o3,m,o2,o1) T2(o1,o2,v2,v1) V2(o3,a,v2,v1)
          19: (
                           1.00000000) D2(i,k,o2,o1) T2(o2,o1,v2,v1) V2(m,a,v2,v1)
          20 : (
                          1.00000000) D3(i,k,o1,m,o2,o3) T2(o2,o3,v1,v2) V2(o1,a,v2,v1)
          21 : (
                           1.00000000) D2(i,k,o1,o2) T2(o2,o1,v1,v2) V2(m,a,v2,v1)
    < RESULT2 >
         0: (1.00000000) D3(i,m,k,o2,o3,o1) T2(o1,o2,v1,a) h(o3,v1)
                          1.00000000) D2(i,o2,k,o1) T2(o2,o1,v1,a) h(m,v1)
           1: (
       2 : (
                          1.00000000) D3(i,m,k,o2,o1,o3) T2(o2,o3,a,v1) h(o1,v1)
                          1.00000000) D2(i,o1,k,o2) T2(o2,o1,a,v1) h(m,v1)
         4: (
                          2.00000000) D3(i,m,k,o2,o3,o1) T2(o1,o2,v1,a) V2(c1,c1,o3,v1)
        5 : (
                          2.00000000) D2(i,o2,k,o1) T2(o2,o1,v1,a) V2(c1,c1,m,v1)
         6: ( 2.00000000) D3(i,m,k,o2,o3,o1) T2(o2,o1,a,v1) V2(c1,c1,m,v1)
7: ( 2.00000000) D2(i,o2,k,o1) T2(o1,o2,a,v1) V2(c1,c1,m,v1)
8: ( -1.00000000) D3(i,m,k,o2,o3,o1) T2(o1,o2,v1,a) V2(c1,o3,c1,v1)
9: ( -1.00000000) D2(i,o2,k,o1) T2(o2,o1,v1,a) V2(c1,m,c1,v1)
9: ( -1.00000000) D2(i,o2,k,o1) T2(o2,o1,v1,a, v2(c1,m,c1,v1, 10: ( -1.00000000) D3(i,m,k,o2,o3,o1) T2(o2,o1,a,v1) V2(c1,o3,c1,v1) 11: ( -1.00000000) D2(i,o2,k,o1) T2(o1,o2,a,v1) V2(c1,m,c1,v1) 12: ( 1.00000000) D4(i,m,k,o3,o4,o1,o5,o2) T2(o1,o3,v1,a) V2(o2,o5,o2) V2(o2,o3,o2) V2(o2,o5,o2) V2(o2,o3,o2) V2(o2,o2,o2) 
      12 : (1.00000000) D4(i,m,k,o3,o4,o1,o5,o2) T2(o1,o3,v1,a) V2(o2,o5,o4,v1)
      13 : (
14 : (
15 : (
                          1.00000000) D3(i,o3,k,o2,o4,o1) T2(o1,o2,v1,a) V2(m,o3,o4,v1)
                          1.00000000) D3(i,o3,k,o2,o4,o1) T2(o3,o2,v1,a) V2(m,v1,o1,o4)
                          1.00000000) D4(i,m,k,o3,o1,o4,o2,o5) T2(o3,o4,a,v1) V2(o1,v1,o2,o5)
                           1.00000000) D3(i,o3,k,o2,o4,o1) T2(o2,o1,a,v1) V2(m,o3,o4,v1)
                          1.00000000) D3(i,o3,k,o2,o4,o1) T2(o2,o3,a,v1) V2(m,v1,o1,o4)
      17 : (
      18 : (
19 : (
20 : (
                          1.00000000) D3(i,m,k,o2,o3,o1) T2(o1,o2,v2,v1) V2(o3,v2,a,v1)
                          1.00000000) D2(i,o2,k,o1) T2(o2,o1,v2,v1) V2(m,v2,a,v1)
                          1.00000000) D3(i,m,k,o2,o1,o3) T2(o2,o3,v1,v2) V2(o1,v2,a,v1)
      21 : ( 1.00000000) D2(i,o1,k.o2) T2(o2,o1,v1,v2) V2(m,v2,a,v1)
     < RESULT >
```

```
eclipse sort.dat
 9 11, 12 16:46
                                                             Page 79/145
            1.00000000) D3(i,m,k,o2,o3,o1) T2(o1,o2,v1,a) h(o3,v1)
   0: (
           1.00000000) D2(i,o2,k,o1) T2(o2,o1,v1,a) h(m,v1)
   1: (
   2: (
           1.00000000) D3(i,m,k,o2,o1,o3) T2(o2,o3,a,v1) h(o1,v1)
   3: (
           1.00000000) D2(i,01,k,02) T2(02,01,a,v1) h(m,v1)
   4: (
           2.00000000) D3(i,m,k,o2,o3,o1) T2(o1,o2,v1,a) V2(c1,c1,o3,v1)
   5 : (
            2.00000000) D2(i,o2,k,o1) T2(o2,o1,v1,a) V2(c1,c1,m,v1)
   6: (
           2.00000000) D3(i,m,k,o2,o3,o1) T2(o2,o1,a,v1) V2(c1,c1,o3,v1)
           2.00000000) D2(i,o2,k,o1) T2(o1,o2,a,v1) V2(c1,c1,m,v1)
   7: (
   8: (
           -1.00000000) D3(i,m,k,o2,o3,o1) T2(o1,o2,v1,a) V2(c1,o3,c1,v1)
          -1.00000000) D2(i,o2,k,o1) T2(o2,o1,v1,a) V2(c1,m,c1,v1)
   9: (
  10: (
          -1.00000000) D3(i,m,k,o2,o3,o1) T2(o2,o1,a,v1) V2(c1,o3,c1,v1)
  11: (
           -1.00000000) D2(i,o2,k,o1) T2(o1,o2,a,v1) V2(c1,m,c1,v1)
  12: (
           1.00000000) D4(i,m,k,o3,o4,o1,o5,o2) T2(o1,o3,v1,a) V2(o2,o5,o4,v1)
           14: (
  15 : (
           1.00000000) D4(i,m,k,03,01,04,02,05) T2(03,04,a,v1) V2(01,v1,02,05)
           1.00000000) D3(i,o3,k,o2,o4,o1) T2(o2,o1,a,v1) V2(m,o3,o4,v1)
  17 : ( 1.00000000) D3(i,o3,k,o2,o4,o1) T2(o2,o3,a,v1) V2(m,v1,o1,o4)
  18 : (
           1.00000000) D3(i,m,k,o2,o3,o1) T2(o1,o2,v2,v1) V2(o3,v2,a,v1)
  19: (
           1.00000000) D2(i,o2,k,o1) T2(o2,o1,v2,v1) V2(m,v2,a,v1)
  20 : (
           1.00000000) D3(i,m,k,o2,o1,o3) T2(o2,o3,v1,v2) V2(o1,v2,a,v1)
  21 : ( 1.00000000) D2(i,o1,k,o2) T2(o2,o1,v1,v2) V2(m,v2,a,v1)
Setting up parameters as default ....
 __/\\\\\\\
 _____/\\\\\\\_\/\\\_\//\\\_\/\\\
                  ____\//\\////_\/_\\\_\/\\\_\/\\\_\/\\\_\/\\\_\
                  _____\//\\\\\\_\/\\\_\/\\\_\/\\\
                    ____\////////__\///__\///__\///___\///___\///___
! * 8 terms are replaced in the linking process ....
The linked formulas ...
0 : ( 1.00000000) D3(i,m,k,o2,o3,o1) T2(o1,o2,v1,a) h(o3,v1)
1: ( 1.00000000) D2(i,o2,k,o1) T2(o2,o1,v1,a) h(m,v1)
2: ( 1.00000000) D3(i,m,k,o2,o1,o3) T2(o2,o3,a,v1) h(o1,v1)
       1.00000000) D2(i,o1,k,o2) T2(o2,o1,a,v1) h(m,v1)
3: (
        2.00000000) D3(i,m,k,o2,o3,o1) T2(o1,o2,v1,a) Y0(o3,v1) 2.00000000) D2(i,o2,k,o1) T2(o2,o1,v1,a) Y1(m,v1)
5 : (
        2.00000000) D3(i,m,k,o2,o3,o1) T2(o2,o1,a,v1) Y2(o3,v1)
6: (
       2.00000000) D2(i,o2,k,o1) T2(o1,o2,a,v1) Y3(m,v1)
7: (
8 : (-1.00000000) D3(i,m,k,o2,o3,o1) T2(o1,o2,v1,a) Y4(o3,v1)
9 : ( -1.00000000) D2(i,o2,k,o1) T2(o2,o1,v1,a) Y5(m,v1)
10 : (-1.00000000) D3(i,m,k,o2,o3,o1) T2(o2,o1,a,v1) Y6(o3,v1)
11 : (-1.00000000) D2(i,o2,k,o1) T2(o1,o2,a,v1) Y7(m,v1)
12: ( 1.00000000) D4(i,m,k,o3,o4,o1,o5,o2) T2(o1,o3,v1,a) V2(o2,o5,o4,v1)
13 : (
        1.00000000) D3(i,o3,k,o2,o4,o1) T2(o1,o2,v1,a) V2(m,o3,o4,v1) 1.00000000) D3(i,o3,k,o2,o4,o1) T2(o3,o2,v1,a) V2(m,v1,o1,o4)
14: (
15 : (
        1.00000000) D4(i,m,k,o3,o1,o4,o2,o5) T2(o3,o4,a,v1) V2(o1,v1,o2,o5)
16: (
         1.00000000) D3(i,o3,k,o2,o4,o1) T2(o2,o1,a,v1) V2(m,o3,o4,v1)
17: (
         1.00000000) D3(i,o3,k,o2,o4,o1) T2(o2,o3,a,v1) V2(m,v1,o1,o4)
         1.00000000) D3(i,m,k,o2,o3,o1) T2(o1,o2,v2,v1) V2(o3,v2,a,v1)
18: (
```

```
eclipse sort.dat
  9 11, 12 16:46
                                                                    Page 80/145
 19 : (
          1.00000000) D2(i,o2,k,o1) T2(o2,o1,v2,v1) V2(m,v2,a,v1)
20 : (1.00000000) D3(i,m,k,o2,o1,o3) T2(o2,o3,v1,v2) V2(o1,v2,a,v1)
21 : (
          1.00000000) D2(i,o1,k,o2) T2(o2,o1,v1,v2) V2(m,v2,a,v1)
The content of each effective tensor ....
Y0 <-- ( 1.00000000) V2(c1,c1,o3,v1)
Y1 <-- (
           1.00000000) V2(c1,c1,m,v1)
Y2 <-- (
           1.00000000) V2(c1,c1,o3,v1)
Y3 <-- (
            1.00000000) V2(c1,c1,m,v1)
1.00000000) V2(c1,o3,c1,v1)
Y4 <-- (
           1.00000000) V2(c1,m,c1,v1)
Y5 <-- (
Y6 <-- ( 1.00000000) V2(c1,o3,c1,v1)
Y7 <-- ( 1.00000000) V2(c1,m,c1,v1)
! No.0
! S2(i,k,m,a) <--
! ( 1.00000000) D3(i,m,k,o2,o3,o1) T2(o1,o2,v1,a) h(o3,v1)
! Indices of BareAmp are rotated to match with LHS.
Case 0 ..... X(i,m,k,o3,v1,a) < ---- (1.00000000) D3(i,m,k,o2,o3,o1) T2(o1
 ! Polynomial order is O(o^6v^2)
! Maximum memory usage is O(o^4v^1)
Case 1 ..... X(i,m,k,o2,o1,v1) < ---- ( 1.00000000) D3(i,m,k,o2,o3,o1) h(o3)
! Polynomial order is O(o^5v^2)
! Maximum memory usage is O(o^5v^1)
Case 2 ..... X(o1,o2,o3,a) <---- ( 1.00000000) T2(o1,o2,v1,a) h(o3,v1)
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^3)
! The optimal choice is .....
1: X(o1,o2,o3,a) <-- ( 1.00000000) T2(o1,o2,v1,a) h(o3,v1)
2: S2(i,k,m,a) <-- ( 1.00000000) D3(i,m,k,o2,o3,o1) X(o1,o2,o3,a)
! Scaling : 0(o^6v^1)
! Max size of X : o^3
! * Begin scaling analysis .... *
for a in {vir}:
 Read T2 from GA for a
  Read S2 from GA for a
  Declare X as a o^3 tensor
  X_{(a)}(o1,o2,o3) += 1.0 sum(v1) T2(o1,o2,v1,) * h(o3,v1)
  S2_{(a)}(i,k,m) += 1.0 sum(02,03,01) D3(i,m,k,02,03,01) * X_{(a)}(01,02,03,)
  Accumulate S2_(a)(i,k,m) for a
! No.1
! S2(i,k,m,a) <--
! ( 1.00000000) D2(i,o2,k,o1) T2(o2,o1,v1,a) h(m,v1)
! Indices of BareAmp are rotated to match with LHS.
Case 0 ..... X(i,k,v1,a) < ---- (1.00000000) D2(i,o2,k,o1) T2(o2,o1,v1,a)
! Polynomial order is O(o^4v^2)
! Maximum memory usage is O(o^2v^1)
Case 1 .... X(i,02,k,01,m,v1) < ---- ( 1.00000000) D2(i,02,k,01) h(m,v1)
 ! Polynomial order is O(o^5v^2)
 ! Maximum memory usage is O(o^5v^1)
Case 2 .... X(o2,o1,m,a) <---- ( 1.00000000) T2(o2,o1,v1,a) h(m,v1)
! Polynomial order is O(o^5v^1)
! Maximum memory usage is O(o^3)
! The optimal choice is .....
```

```
eclipse sort.dat
 9 11, 12 16:46
                                                                    Page 81/145
1: X(02,01,m,a) < -- (1.00000000) T2(02,01,v1,a) h(m,v1)
2: S2(i,k,m,a) < -- ( 1.00000000) D2(i,o2,k,o1) X(o2,o1,m,a)
              : O(o^5v^1)
! Max size of X : o^3
! * Begin scaling analysis .... *
for a in {vir}:
 Read T2 from GA for a
 Read S2 from GA for a
 Declare X as a o^3 tensor
 X (a)(o2,o1,m) += 1.0 sum(v1) T2(o2,o1,v1,) * h(m,v1)
 S2_{(a)}(i,k,m) += 1.0 sum(o2,o1) D2(i,o2,k,o1) * X_{(a)}(o2,o1,m,)
 Accumulate S2 (a)(i,k,m) for a
! S2(i,k,m,a) <--
! ( 1.00000000) D3(i,m,k,o2,o1,o3) T2(o2,o3,a,v1) h(o1,v1)
Case 0 ..... X(i,m,k,o1,a,v1) < ---- (1.00000000) D3(i,m,k,o2,o1,o3) T2(o2)
,o3,a,v1)
! Polynomial order is O(o^6v^2)
! Maximum memory usage is O(o^4)
Case 1 .... X(i,m,k,o2,o3,v1) <---- ( 1.00000000) D3(i,m,k,o2,o1,o3) h(o1
! Polynomial order is O(o^5v^2)
! Maximum memory usage is O(o^5)
Case 2 ..... X(02,03,01,a) < ---- ( 1.00000000) T2(02,03,a,v1) h(01,v1)
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^3)
! The optimal choice is .....
1: X(02,03,01,a) < -- ( 1.00000000) T2(02,03,a,v1) h(01,v1) 2: S2(i,k,m,a) < -- ( 1.00000000) D3(i,m,k,o2,o1,o3) X(o2,o3,o1,a)
! Scaling
              : O(o^6v^1)
! Max size of X : o^3
! * Begin scaling analysis .... *
for a in {vir}:
 Read S2 from GA for a
 Declare X as a o^3 tensor
 for v1 in {vir}:
   Read T2 from GA for v1
   X_{(a)}(o2,o3,o1) += 1.0 sum() T2(o2,o3,a,) * h(o1,v1)
 S2_{(a)}(i,k,m) += 1.0 sum(02,01,03) D3(i,m,k,02,01,03) * X_{(a)}(02,03,01,)
 Accumulate S2_(a)(i,k,m) for a
! S2(i,k,m,a) <--
! ( 1.00000000) D2(i,o1,k,o2) T2(o2,o1,a,v1) h(m,v1)
Case 0 ..... X(i,k,a,v1) < ---- (1.00000000) D2(i,o1,k,o2) T2(o2,o1,a,v1)
! Polynomial order is O(o^4v^2)
! Maximum memory usage is O(o^2)
Case 1 ..... X(i,01,k,02,m,v1) < ---- (1.00000000) D2(i,01,k,02) h(m,v1)
! Polynomial order is O(o^5v^2)
```

```
eclipse sort.dat
    9 11, 12 16:46
                                                                                                                                                 Page 82/145
 ! Maximum memory usage is O(o^5)
Case 2 ..... X(02,01,m,a) < ---- ( 1.00000000) T2(02,01,a,v1) h(m,v1)
 ! Polynomial order is O(o^5v^1)
 ! Maximum memory usage is O(o^3)
Factorize: Conflict between choices of optimal memory usage and polynomial order
! The optimal choice is .....
1: X(02,01,m,a) < -- ( 1.00000000) T2(02,01,a,v1) h(m,v1) 2: S2(i,k,m,a) < -- ( 1.00000000) D2(i,01,k,02) X(02,01,m,a)
! Scaling
                            : O(o^5v^1)
! Max size of X : o^3
 ! * Begin scaling analysis .... *
for a in {vir}:
   Read S2 from GA for a
    Declare X as a o^3 tensor
    for v1 in {vir}:
       Read T2 from GA for v1
       X_{(a)(o2,o1,m)} += 1.0 sum() T2(o2,o1,a,) * h(m,v1)
    S2_{(a)}(i,k,m) += 1.0 sum(o1,o2) D2(i,o1,k,o2) * X_{(a)}(o2,o1,m,)
    Accumulate S2_(a)(i,k,m) for a
! S2(i,k,m,a) <--
! ( 2.00000000) D3(i,m,k,o2,o3,o1) T2(o1,o2,v1,a) Y0(o3,v1)
! Indices of BareAmp are rotated to match with LHS.
Case 0 ..... X(i,m,k,o3,v1,a) < ---- ( 1.00000000) D3(i,m,k,o2,o3,o1) T2(o1) D3(i,m,k,o2,o3,o1) T2(o1) D3(i,m,k,o2,o3,o1) D3(i,m,k,o2,o1) D3(i,m,k,o1) D3(i,m,k,o2,o1) D3(i,m,k,o2,o1) D3(i,m,k,o2,o1) D3(i,m,k,o2,o
,o2,v1,a)
! Polynomial order is O(o^6v^2)
! Maximum memory usage is O(o^4v^1)
Case 1 .... X(i,m,k,o2,o1,v1) < ---- (1.00000000) D3(i,m,k,o2,o3,o1) Y0(o
3.v1)
! Polynomial order is O(o^5v^2)
! Maximum memory usage is O(o^5v^1)
Case 2 ..... X(01,02,03,a) < ---- (1.00000000) T2(01,02,v1,a) Y0(03,v1)
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^3)
! The optimal choice is .....
1: X(o1,o2,o3,a) <-- ( 1.00000000) T2(o1,o2,v1,a) Y0(o3,v1)
2: S2(i,k,m,a) <-- ( 2.00000000) D3(i,m,k,o2,o3,o1) X(o1,o2,o3,a)
 ! Scaling
                               : O(o^6v^1)
! Max size of X : o^3
! * Begin scaling analysis .... *
Declare Y0 as a tensor
for c1 in {core}:
   Read V2 from GA for c1
for a in {vir}:
    Read T2 from GA for a
    Read S2 from GA for a
    Declare X as a o^3 tensor
    X_{(a)}(01,02,03) += 1.0 sum(v1) T2(01,02,v1,) * Y0(03,v1)
     S2_{(a)}(i,k,m) += 2 sum(o2,o3,o1) D3(i,m,k,o2,o3,o1) * X_{(a)}(o1,o2,o3,)
    Accumulate S2_(a)(i,k,m) for a
```

```
eclipse_sort.dat
   9 11, 12 16:46
                                                                                                                                                 Page 83/145
! No.5
! S2(i,k,m,a) <--
! ( 2.00000000) D2(i,o2,k,o1) T2(o2,o1,v1,a) Y1(m,v1)
! Indices of BareAmp are rotated to match with LHS.
Case 0 ..... X(i,k,v1,a) < ---- (1.00000000) D2(i,o2,k,o1) T2(o2,o1,v1,a)
! Polynomial order is O(o^4v^2)
! Maximum memory usage is O(o^2v^1)
Case 1 ..... X(i,o_2,k,o_1,m,v_1) < ---- ( 1.00000000) D2(i,o_2,k,o_1) Y1(m,v_1)
! Polynomial order is O(o^5v^2)
! Maximum memory usage is O(o^5v^1)
Case 2 ..... X(02,01,m,a) < ---- ( 1.00000000) T2(02,01,v1,a) Y1(m,v1)
! Polynomial order is O(o^5v^1)
! Maximum memory usage is O(o^3)
! The optimal choice is .....
1: X(o2,o1,m,a) < -- ( 1.00000000) T2(o2,o1,v1,a) Y1(m,v1) 2: S2(i,k,m,a) < -- ( 2.00000000) D2(i,o2,k,o1) X(o2,o1,m,a)
! Scaling
                             : O(o^5v^1)
! Max size of X : o^3
! * Begin scaling analysis .... *
Declare Y1 as a tensor
for c1 in {core}:
   Read V2 from GA for c1
for a in {vir}:
   Read T2 from GA for a
   Read S2 from GA for a
   Declare X as a o^3 tensor
   X (a)(o2,o1,m) += 1.0 sum(v1) T2(o2,o1,v1,) * Y1(m,v1)
   S2_{(a)}(i,k,m) += 2 sum(o2,o1) D2(i,o2,k,o1) * X_{(a)}(o2,o1,m,)
   Accumulate S2_(a)(i,k,m) for a
! S2(i,k,m,a) <--
! (2.00000000) D3(i,m,k,o2,o3,o1) T2(o2,o1,a,v1) Y2(o3,v1)
Case 0 ..... X(i,m,k,o3,a,v1) < ---- ( 1.00000000) D3(i,m,k,o2,o3,o1) T2(o2) D3(i,m,k,o2,o3,o1) T2(o2) D3(i,m,k,o3,a,v1) C3(i,m,k,o3,a,v1) C3(i,m,k,o3,a,v
,o1,a,v1)
! Polynomial order is O(o^6v^2)
! Maximum memory usage is O(o^4)
Case 1 ..... X(i,m,k,o2,o1,v1) <---- ( 1.00000000) D3(i,m,k,o2,o3,o1) Y2(o
3,v1)
! Polynomial order is O(o^5v^2)
! Maximum memory usage is O(o^5)
Case 2 ..... X(0.2,0.1,0.3,a) < ---- ( 1.00000000) T2(0.2,0.1,a,v.1) Y2(0.3,v.1)
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^3)
! The optimal choice is .....
1: X(o2,o1,o3,a) <-- ( 1.00000000) T2(o2,o1,a,v1) Y2(o3,v1)
2: S2(i,k,m,a) <-- ( 2.00000000) D3(i,m,k,o2,o3,o1) X(o2,o1,o3,a)
! Scaling
                              : O(o^6v^1)
! Max size of X : o^3
! * Begin scaling analysis .... *
```

9 11, 12 16:46	eclipse_sort.dat	Page 84/145
Declare Y2 as a tensor for c1 in {core}: Read V2 from GA for c1		
for a in {vir}: Read S2 from GA for a Declare X as a o^3 tensor for v1 in {vir}: Read T2 from GA for v1 X_(a)(o2,o1,o3) += 1.0 su	um() T2(o2,o1,a,) * Y2(o3,v1)	
S2_(a)(i,k,m) += 2 sum(o2,o	o3,o1) D3(i,m,k,o2,o3,o1) * X_(a)	(02,01,03,)
Accumulate S2_(a)(i,k,m) fo	or a	
!		
! Polynomial order is O(o^4v^ ! Maximum memory usage is O(o Case 1 X(i,o2,k,o1,m,v1 ! Polynomial order is O(o^5v^ ! Maximum memory usage is O(o Case 2 X(o1,o2,m,a) <- ! Polynomial order is O(o^5v^ ! Maximum memory usage is O(o	(1.00000000) D2(i,o2,k, '2) '^2) (1.00000000) D2(i '2) (1.00000000) T2(o1,o2, '1)	a,v1) Y3(m,v1)
! The optimal choice is 1: X(o1,o2,m,a) < (1. 2: S2(i,k,m,a) < (2.0	00000000) T2(o1,o2,a,v1) Y3(m,v 0000000) D2(i,o2,k,o1) X(o1,o2,m	r1) n,a)
! Scaling : O(o^5v^1) ! Max size of X : o^3		
! * Begin scaling analysis	*	
Declare Y3 as a tensor for c1 in {core}: Read V2 from GA for c1		
for a in {vir}: Read S2 from GA for a Declare X as a o^3 tensor for v1 in {vir}: Read T2 from GA for v1 X_(a)(01,02,m) += 1.0 sum	n() T2(o1,o2,a,) * Y3(m,v1)	
S2_(a)(i,k,m) += 2 sum(o2,o	ol) D2(i,o2,k,o1) * X_(a)(o1,o2,m	1,)
Accumulate S2_(a)(i,k,m) fo	or a	
!		
! No.8 ! S2(i,k,m,a) < ! (-1.00000000) D3(i,m,k,o ! Indices of BareAmp are rota Case 0 X(i,m,k,o3,v1,a) ,o2,v1,a)		m,k,o2,o3,o1) T2(o1

```
eclipse sort.dat
 9 11, 12 16:46
                                                                      Page 85/145
! Polynomial order is O(o^6v^2)
! Maximum memory usage is O(o^4v^1)
Case 1 ..... X(i,m,k,o2,o1,v1) < ---- (1.00000000) D3(i,m,k,o2,o3,o1) Y4(o
3,v1)
! Polynomial order is O(o^5v^2)
! Maximum memory usage is O(o^5v^1)
Case 2 ..... X(01,02,03,a) < ---- ( 1.00000000) T2(01,02,v1,a) Y4(03,v1)
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^3)
! The optimal choice is .....
1: X(o1,o2,o3,a) <-- ( 1.00000000) T2(o1,o2,v1,a) Y4(o3,v1)
2: S2(i,k,m,a) <-- ( -1.00000000) D3(i,m,k,o2,o3,o1) X(o1,o2,o3,a)
! Scaling
              : O(o^6v^1)
! Max size of X : o^3
! * Begin scaling analysis .... *
Declare Y4 as a tensor
for c1 in {core}:
 Read V2 from GA for c1
for a in {vir}:
 Read T2 from GA for a
 Read S2 from GA for a
 Declare X as a o^3 tensor
 X (a)(01,02,03) += 1.0 sum(v1) T2(01,02,v1,) * Y4(03,v1)
 S2_{(a)}(i,k,m) += -1 sum(o2,o3,o1) D3(i,m,k,o2,o3,o1) * X_{(a)}(o1,o2,o3,)
 Accumulate S2_(a)(i,k,m) for a
! S2(i,k,m,a) <--
! ( -1.00000000) D2(i.o2.k.o1) T2(o2.o1.v1.a) Y5(m.v1)
! Indices of BareAmp are rotated to match with LHS.
Case 0 ..... X(i,k,v1,a) < ---- (1.00000000) D2(i,o2,k,o1) T2(o2,o1,v1,a)
! Polynomial order is O(o^4v^2)
! Maximum memory usage is O(o^2v^1)
Case 1 ..... X(i,02,k,01,m,v1) < ---- (1.00000000) D2(i,02,k,01) Y5(m,v1)
! Polynomial order is O(o^5v^2)
! Maximum memory usage is O(o^5v^1)
Case 2 ..... X(o2,o1,m,a) <---- ( 1.00000000) T2(o2,o1,v1,a) Y5(m,v1)
! Polynomial order is O(o^5v^1)
! Maximum memory usage is O(o^3)
! The optimal choice is .....
1: X(02,01,m,a) <-- ( 1.00000000) T2(02,01,v1,a) Y5(m,v1)
2: S2(i,k,m,a) <-- ( -1.00000000) D2(i,02,k,01) X(02,01,m,a)
! Scaling
              : O(o^5v^1)
! Max size of X : o^3
! * Begin scaling analysis .... *
Declare Y5 as a tensor
for c1 in {core}:
 Read V2 from GA for c1
for a in {vir}:
 Read T2 from GA for a
 Read S2 from GA for a
 Declare X as a o^3 tensor
 X_{(a)}(o2,o1,m) += 1.0 sum(v1) T2(o2,o1,v1,) * Y5(m,v1)
```

```
eclipse sort.dat
    9 11, 12 16:46
                                                                                                                                            Page 86/145
    S2_{(a)}(i,k,m) += -1 sum(o2,o1) D2(i,o2,k,o1) * X_{(a)}(o2,o1,m,)
    Accumulate S2 (a)(i,k,m) for a
! S2(i,k,m,a) <--
! ( -1.00000000) D3(i,m,k,o2,o3,o1) T2(o2,o1,a,v1) Y6(o3,v1)
Case 0 ..... X(i,m,k,o3,a,v1) < ---- ( 1.00000000) D3(i,m,k,o2,o3,o1) T2(o2) D3(i,m,k,o2,o3,o1) T2(o2) D3(i,m,k,o3,o3,o1) D3(i,m,k,o2,o3,o1) D3(i,m,k,o3,o3,o1) D3(i,m,k,o3,o1) D3(i,m,k,o1) D3(i,m,
! Polynomial order is O(o^6v^2)
 ! Maximum memory usage is O(o^4)
Case 1 ..... X(i,m,k,o2,o1,v1) <---- ( 1.00000000) D3(i,m,k,o2,o3,o1) Y6(o
3.v1)
! Polynomial order is O(o^5v^2)
! Maximum memory usage is O(o^5)
Case 2 ..... X(02,01,03,a) < ---- ( 1.00000000) T2(02,01,a,v1) Y6(03,v1)
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^3)
! The optimal choice is .....
1: X(02,01,03,a) < -- ( 1.00000000) T2(02,01,a,v1) Y6(03,v1) 2: S2(i,k,m,a) < -- ( -1.00000000) D3(i,m,k,o2,o3,o1) X(o2,o1,o3,a)
 ! Scaling
                             : O(o^6v^1)
! Max size of X : o^3
! * Begin scaling analysis .... *
Declare Y6 as a tensor
for c1 in {core}:
   Read V2 from GA for c1
for a in {vir}:
    Read S2 from GA for a
    Declare X as a o^3 tensor
    for v1 in {vir}:
      Read T2 from GA for v1
       X (a)(o2,o1,o3) += 1.0 sum() T2(o2,o1,a,) * Y6(o3,v1)
    S2_{(a)}(i,k,m) += -1 sum(02,03,01) D3(i,m,k,02,03,01) * X_{(a)}(02,01,03,)
    Accumulate S2_(a)(i,k,m) for a
! No.11
! S2(i,k,m,a) <--
! ( -1.00000000) D2(i,o2,k,o1) T2(o1,o2,a,v1) Y7(m,v1)
Case 0 ..... X(i,k,a,v1) < ---- ( 1.00000000) D2(i,o2,k,o1) T2(o1,o2,a,v1)
! Polynomial order is O(o^4v^2)
! Maximum memory usage is O(o^2)
Case 1 .... X(i,02,k,01,m,v1) < ---- (1.00000000) D2(i,02,k,01) Y7(m,v1)
! Polynomial order is O(o^5v^2)
! Maximum memory usage is O(o^5)
Case 2 ..... X(o1,o2,m,a) < ---- ( 1.00000000) T2(o1,o2,a,v1) Y7(m,v1)
! Polynomial order is O(o^5v^1)
! Maximum memory usage is O(o^3)
Factorize: Conflict between choices of optimal memory usage and polynomial order
! The optimal choice is .....
1: X(o1,o2,m,a) < -- ( 1.00000000) T2(o1,o2,a,v1) Y7(m,v1)
```

```
eclipse sort.dat
  9 11, 12 16:46
                                                                       Page 87/145
2: S2(i,k,m,a) < --  (
                         -1.00000000) D2(i,o2,k,o1) X(o1,o2,m,a)
! Scaling
              : O(o^5v^1)
! Max size of X : o^3
! * Begin scaling analysis .... *
Declare Y7 as a tensor
for c1 in {core}:
  Read V2 from GA for c1
for a in {vir}:
  Read S2 from GA for a
  Declare X as a o^3 tensor
  for v1 in {vir}:
    Read T2 from GA for v1
    X_{(a)}(o1,o2,m) += 1.0 sum() T2(o1,o2,a,) * Y7(m,v1)
  S2_{(a)(i,k,m)} += -1 sum(o2,o1) D2(i,o2,k,o1) * X_{(a)(o1,o2,m,)}
  Accumulate S2 (a)(i,k,m) for a
! No.12
! S2(i,k,m,a) <--
! ( 1.00000000) D4(i,m,k,o3,o4,o1,o5,o2) T2(o1,o3,v1,a) V2(o2,o5,o4,v1)
! Indices of BareAmp are rotated to match with LHS.
! Indices of ERI and D4 are rotated to match with each other.
H2: 0 D4: 37
*TEST* ( 1.00000000) D4(o2,o5,m,i,o3,k,o1,o4) T2(o1,o3,v1,a) V2(o2,o5,o4,v1)
! *** D4(02,05,m,i,03,k,01,04) T2(01,03,v1,a) is skipped due to the priority
Case 1 ..... X(m,i,o3,k,o1,v1) < ---- (1.00000000) D4(o2,o5,m,i,o3,k,o1,o4)
) V2(o2,o5,o4,v1)
! Polynomial order is O(o^8v^1)
! Maximum memory usage is O(o^5v^1)
Case 2 ..... X(o1,o3,o2,o5,o4,a) <---- ( 1.00000000) T2(o1,o3,v1,a) V2(o2,
o5.o4.v1)
! Polynomial order is O(o^8v^1)
! Maximum memory usage is O(o^3)
! Case 0 is skipped due to the priority of ERI ....
! The optimal choice is .....
1: X(o1,o3,o2,o5,o4,a) <-- ( 1.00000000) T2(o1,o3,v1,a) V2(o2,o5,o4,v1) 2: S2(i,k,m,a) <-- ( 1.0000000) D4(o2,o5,m,i,o3,k,o1,o4) X(o1,o3,o2,o5,o4,
a)
! Scaling
              : O(o^8v^1)
! Max size of X : o^3
! * Begin scaling analysis .... *
for o2 in {occ}:
 Read V2 from GA for o2
  for o5 in {occ}:
    Read D4 from GA for o2, o5
    for a in {vir}:
      Read T2 from GA for a
      Read S2 from GA for a
      Declare X as a o^3 tensor
      X_{(02,05,a)}(01,03,04) += 1.0 \text{ sum}(v1) V2(,05,04,v1) * T2(01,03,v1,)
      S2_{(a)}(i,k,m) += 1.0 \text{ sum}(03,01,04) D4(,,m,i,03,k,01,04) * X_{(02,05,a)}(01,0)
3,,,04,)
      Accumulate S2_(a)(i,k,m) for a
```

9 11, 12 16:46	eclipse_sort.dat	Page 88/145
!		
! Indices of BareAmp are rotat ! The indices of ERI are rotat ! *** D3(i,o3,k,o2,o4,o1) T2(o Case 1 X(i,k,o2,o1,m,v1) v1,o4,m,o3) ! Polynomial order is O(o^7v^1 ! Maximum memory usage is O(o^	ed to became virtual. 1,02,v1,a) is skipped due to t < (1.00000000) D3(i) 5)) < (1.00000000) T2()	he priority ,,o3,k,o2,o4,o1) V2(
	1.00000000) D3(i,o3,k,o2,o4, 000000) T2(o1,o2,v1,a) X(i,k,o2	
! Scaling : O(o^7v^1) ! Max size of X : o^5		
! * Begin scaling analysis	. *	
for a in {vir}: Read S2 from GA for a Read T2 from GA for a	um(o4,o3) V2(,o4,m,o3) * D3(i,o	
Accumulate S2_(a)(i,k,m) f	or a	
!		
! Indices of BareAmp are rotat ! The indices of ERI are rotat ! *** D3(i,o3,k,o2,o4,o1) T2(o Case 1 X(i,o3,k,o2,m,v1) v1,m,o1,o4) ! Polynomial order is O(o^7v^1 ! Maximum memory usage is O(o^	ed to became virtual. 3,02,v1,a) is skipped due to t < (1.00000000) D3(i) 5)) < (1.00000000) T2()	he priority ,,03,k,02,04,01) V2(
! The optimal choice is 1: X(i,o3,k,o2,m,v1) < (2: S2(i,k,m,a) < (1.00	1.00000000) D3(i,o3,k,o2,o4, 000000) T2(o3,o2,v1,a) X(i,o3,k	o1) V2(v1,m,o1,o4)
! Scaling : O(o^7v^1) ! Max size of X : o^5		
! * Begin scaling analysis	. *	
for v1 in {vir}:		

```
eclipse_sort.dat
   9 11, 12 16:46
                                                                                                                                        Page 89/145
   Read V2 from GA for v1
   Declare X as a o^5 tensor
   X_{(v1)(i,o3,k,o2,m)} += 1.0 sum(o1,o4) V2(,m,o1,o4) * D3(i,o3,k,o2,o4,o1)
   for a in {vir}:
       Read S2 from GA for a
        Read T2 from GA for a
        S2_{(a)}(i,k,m) += 1.0 sum(o3,o2) T2(o3,o2,v1,) * X_{(v1)}(i,o3,k,o2,m,)
        Accumulate S2 (a)(i,k,m) for a
! No.15
! S2(i,k,m,a) <--
! ( 1.00000000) D4(i,m,k,o3,o1,o4,o2,o5) T2(o3,o4,a,v1) V2(o1,v1,o2,o5)
! Indices of ERI are rotated to match with Bareamp.
! *** D4(i,m,k,o3,o1,o4,o2,o5) T2(o3,o4,a,v1) is skipped due to the priority
Case 1 ..... X(i,m,k,o3,o4,v1) <---- ( 1.00000000) D4(i,m,k,o3,o1,o4,o2,o5)
) V2(v1,o1,o2,o5)
! Polynomial order is O(o^8v^1)
! Maximum memory usage is O(o^3)
Case 2 ..... X(o3,o4,o1,o2,o5,a) <---- ( 1.00000000) T2(o3,o4,a,v1) V2(v1,
01,02,05)
! Polynomial order is O(o^8v^1)
! Maximum memory usage is O(o^5)
! The optimal choice is .....
1: X(i,m,k,o3,o4,v1) < -- (
                                                              1.00000000) D4(i,m,k,o3,o1,o4,o2,o5) V2(v1,o1,o
2: S2(i,k,m,a) < -- ( 1.00000000) T2(03,04,a,v1) X(i,m,k,03,04,v1)
! Scaling
                            : O(o^8v^1)
! Max size of X : o^3
! * Begin scaling analysis .... *
for v1 in {vir}:
   Read V2 from GA for v1
   Read T2 from GA for v1
   for i in {occ}:
        for m in {occ}:
           Read D4 from GA for i, m
            Declare X as a o^3 tensor
            X_{(v1,i,m)(k,o3,o4)} += 1.0 \text{ sum}(o1,o2,o5) V2(,o1,o2,o5) * D4(,,k,o3,o1,o4,o
2,05)
            for a in {vir}:
               Read S2 from GA for a
               S2_{(a)}(i,k,m) += 1.0 sum(03,04) T2(03,04,a,) * X_{(v1,i,m)}(,,k,03,04,)
               Accumulate S2_(a)(i,k,m) for a
! No.16
! S2(i,k,m,a) <--
! (1.00000000) D3(i,o3,k,o2,o4,o1) T2(o2,o1,a,v1) V2(m,o3,o4,v1)
! Indices of ERI are rotated to match with Bareamp.
! *** D3(i,o3,k,o2,o4,o1) T2(o2,o1,a,v1) is skipped due to the priority
Case 1 ..... X(i,k,o2,o1,m,v1) <---- ( 1.00000000) D3(i,o3,k,o2,o4,o1) V2(
v1,04,m,03)
! Polynomial order is O(o^7v^1)
! Maximum memory usage is O(o^5)
Case 2 ..... X(02,01,04,m,03,a) < ---- ( 1.00000000) T2(02,01,a,v1) V2(v1,0) T2(02,01,a,v1) V2(v1,0) T2(02,01,a,v1) V2(v1,0) T2(02,01,a,v1) V2(v1,0) T2(02,01,a,v1) V2(v1,0) V2(v1,0)
```

9 11, 12 16:46	eclipse_sort.dat	Page 90/145
4,m,o3) ! Polynomial order is O(o^7v^1) ! Maximum memory usage is O(o^!		
! The optimal choice is 1: X(i,k,o2,o1,m,v1) < (2: S2(i,k,m,a) < (1.000	1.00000000) D3(i,o3,k,o2 000000) T2(o2,o1,a,v1) X(i,	2,04,01) V2(v1,04,m,03) k,02,01,m,v1)
! Scaling : O(o^7v^1) ! Max size of X : o^5		
! * Begin scaling analysis	. *	
for v1 in {vir}: Read V2 from GA for v1 Read T2 from GA for v1 Declare X as a o^5 tensor X_(v1)(i,k,o2,o1,m) += 1.0 st	um(o4,o3) V2(,o4,m,o3) * D3	s(i,o3,k,o2,o4,o1)
for a in {vir}: Read S2 from GA for a S2_(a)(i,k,m) += 1.0 sum(o2	2,o1) T2(o2,o1,a,) * X_(v1)	(i,k,o2,o1,m,)
Accumulate S2_(a)(i,k,m) for	or a	
!		
! No.17 ! S2(i,k,m,a) < ! (1.00000000) D3(i,o3,k,o2 ! Indices of ERI are rotated to ! *** D3(i,o3,k,o2,o4,o1) T2(o2 Case 1 X(i,o3,k,o2,m,v1) v1,m,o1,o4) ! Polynomial order is O(o^7v^1 ! Maximum memory usage is O(o^5 Case 2 X(o2,o3,m,o1,o4,a,o1,o4) ! Polynomial order is O(o^7v^1 ! Maximum memory usage is O(o^5)	2,03,a,v1) is skipped due < (1.00000000)) 5) > (1.00000000)	to the priority D3(i,o3,k,o2,o4,o1) V2(
! The optimal choice is 1: X(i,o3,k,o2,m,v1) < (2: S2(i,k,m,a) < (1.000	1.00000000) D3(i,o3,k,o2 000000) T2(o2,o3,a,v1) X(i,	2,04,01) V2(v1,m,01,04) 03,k,02,m,v1)
! Scaling : O(o^7v^1) ! Max size of X : o^5		
! * Begin scaling analysis	. *	
<pre>for v1 in {vir}: Read V2 from GA for v1 Read T2 from GA for v1 Declare X as a o^5 tensor X_(v1)(i,o3,k,o2,m) += 1.0 st</pre>	um(o1,o4) V2(,m,o1,o4) * D3	s(i,o3,k,o2,o4,o1)
for a in {vir}: Read S2 from GA for a S2_(a)(i,k,m) += 1.0 sum(o2	2,03) T2(02,03,a,) * X_(v1)	(i,03,k,02,m,)
Accumulate S2_(a)(i,k,m) for	or a	
!		
! No.18		

```
eclipse sort.dat
 9 11, 12 16:46
                                                                      Page 91/145
! S2(i,k,m,a) <--
! ( 1.00000000) D3(i,m,k,o2,o3,o1) T2(o1,o2,v2,v1) V2(o3,v2,a,v1)
! Indices of ERI are rotated to match with LHS.
! *** D3(i,m,k,o2,o3,o1) T2(o1,o2,v2,v1) is skipped due to the priority
Case 1 ..... X(i,m,k,o2,o1,a,v1,v2) < ---- ( 1.00000000) D3(i,m,k,o2,o3,o1)
V2(a.v1.o3.v2)
! Polynomial order is O(o^6v^3)
! Maximum memory usage is O(o^5v^1)
Case 2 ..... X(01,02,03,a) < ---- (1.00000000) T2(01,02,v2,v1) V2(a,v1,03,000)
! Polynomial order is O(o^3v^3)
! Maximum memory usage is O(o^3)
! The optimal choice is .....
1: X(o1,o2,o3,a) <-- ( 1.00000000) T2(o1,o2,v2,v1) V2(a,v1,o3,v2) 
2: S2(i,k,m,a) <-- ( 1.00000000) D3(i,m,k,o2,o3,o1) X(o1,o2,o3,a)
! Scaling
              : O(o^3v^3)
! Max size of X : o^3
! * Begin scaling analysis .... *
for a in {vir}:
 Read V2 from GA for a
 Read S2 from GA for a
 Declare X as a o^3 tensor
 for v1 in {vir}:
   Read T2 from GA for v1
   X_{(a)}(o1,o2,o3) += 1.0 sum(v2) V2(,v1,o3,v2) * T2(o1,o2,v2,)
 S2(a)(i,k,m) += 1.0 sum(o2,o3,o1) D3(i,m,k,o2,o3,o1) * X(a)(o1,o2,o3,)
 Accumulate S2 (a)(i,k,m) for a
! No.19
! S2(i,k,m,a) <--
! (1.00000000) D2(i,o2,k,o1) T2(o2,o1,v2,v1) V2(m,v2,a,v1)
! Indices of ERI are rotated to match with LHS.
! *** D2(i,o2,k,o1) T2(o2,o1,v2,v1) is skipped due to the priority
Case 1 ..... X(i,o2,k,o1,m,a,v1,v2) < ---- ( 1.00000000) D2(i,o2,k,o1) V2(a)
,v1,m,v2)
! Polynomial order is O(o^5v^3)
! Maximum memory usage is O(o^5v^1)
Case 2 ..... X(02,01,m,a) <---- ( 1.00000000) T2(02,01,v2,v1) V2(a,v1,m,v2
! Polynomial order is O(o^3v^3)
! Maximum memory usage is O(o^3)
! The optimal choice is .....
1: X(02,01,m,a) < -- ( 1.00000000) T2(02,01,v2,v1) V2(a,v1,m,v2) 2: S2(i,k,m,a) < -- ( 1.00000000) D2(i,02,k,01) X(02,01,m,a)
! Scaling
             : O(o^3v^3)
! Max size of X : o^3
! * Begin scaling analysis .... *
for a in {vir}:
 Read V2 from GA for a
 Read S2 from GA for a
 Declare X as a o^3 tensor
 for v1 in {vir}:
   Read T2 from GA for v1
    X_{(a)}(o2,o1,m) += 1.0 sum(v2) V2(,v1,m,v2) * T2(o2,o1,v2,)
```

```
eclipse sort.dat
  9 11. 12 16:46
                                                                      Page 92/145
  S2 (a)(i,k,m) += 1.0 sum(o2,o1) D2(i,o2,k,o1) * X (a)(o2,o1,m,)
  Accumulate S2 (a)(i,k,m) for a
! No.20
! S2(i,k,m,a) <--
! ( 1.00000000) D3(i,m,k,o2,o1,o3) T2(o2,o3,v1,v2) V2(o1,v2,a,v1)
! Indices of ERI are rotated to match with LHS.
! *** D3(i,m,k,o2,o1,o3) T2(o2,o3,v1,v2) is skipped due to the priority
Case 1 ..... X(i,m,k,o2,o3,a,v1,v2) < ---- (1.00000000) D3(i,m,k,o2,o1,o3)
 V2(a,v1,o1,v2)
 ! Polynomial order is O(o^6v^3)
! Maximum memory usage is O(o^5v^1)
Case 2 ..... X(02,03,01,a) < ---- (1.00000000) T2(02,03,v1,v2) V2(a,v1,01,a)
! Polynomial order is O(o^3v^3)
! Maximum memory usage is O(o^3)
! The optimal choice is .....
1: X(o2,o3,o1,a) <-- ( 1.00000000) T2(o2,o3,v1,v2) V2(a,v1,o1,v2) 
2: S2(i,k,m,a) <-- ( 1.00000000) D3(i,m,k,o2,o1,o3) X(o2,o3,o1,a)
! Scaling : O(o^3v^3)
! Max size of X : o^3
! * Begin scaling analysis .... *
for a in {vir}:
  Read V2 from GA for a
  Read S2 from GA for a
  Declare X as a o^3 tensor
  for v2 in {vir}:
   Read T2 from GA for v2
   X (a)(02,03,01) += 1.0 sum(v1) V2(,v1,01,v2) * T2(02,03,v1,)
  S2 (a)(i,k,m) += 1.0 sum(02,01,03) D3(i,m,k,02,01,03) * X_(a)(02,03,01,)
  Accumulate S2 (a)(i,k,m) for a
! No.21
! S2(i,k,m,a) <--
! ( 1.00000000) D2(i,o1,k,o2) T2(o2,o1,v1,v2) V2(m,v2,a,v1)
! Indices of ERI are rotated to match with LHS.
! *** D2(i,o1,k,o2) T2(o2,o1,v1,v2) is skipped due to the priority
Case 1 ..... X(i,o1,k,o2,m,a,v1,v2) <---- ( 1.00000000) D2(i,o1,k,o2) V2(a
,v1,m,v2)
! Polynomial order is O(o^5v^3)
! Maximum memory usage is O(o^5v^1)
Case 2 ..... X(o2,o1,m,a) <---- ( 1.00000000) T2(o2,o1,v1,v2) V2(a,v1,m,v2
! Polynomial order is O(o^3v^3)
! Maximum memory usage is O(o^3)
! The optimal choice is .....
1: X(o2,o1,m,a) <-- ( 1.00000000) T2(o2,o1,v1,v2) V2(a,v1,m,v2) 
2: S2(i,k,m,a) <-- ( 1.00000000) D2(i,o1,k,o2) X(o2,o1,m,a)
! Scaling
              : O(o^3v^3)
! Max size of X : o^3
! * Begin scaling analysis .... *
```

```
eclipse_sort.dat
 9 11, 12 16:46
                                                                     Page 93/145
for a in {vir}:
 Read V2 from GA for a
 Read S2 from GA for a
 Declare X as a o^3 tensor
 for v2 in {vir}:
   Read T2 from GA for v2
   X_{(a)(o2,o1,m)} += 1.0 sum(v1) V2(,v1,m,v2) * T2(o2,o1,v1,)
 S2_{(a)}(i,k,m) += 1.0 \text{ sum}(o1,o2) D2(i,o1,k,o2) * X_{(a)}(o2,o1,m,)
 Accumulate S2_(a)(i,k,m) for a
* 4 <000V/000V>
     0.25000000) T2(o1,o2,o3,a) V2(c1,c2,c3,c4) E5(c1,c2,i,k,o3,c3,c4,m,o2,o1)
    0.25000000) T2(o1,o2,m,a) V2(c1,c2,c3,c4) E4(c1,c2,i,k,c3,c4,o1,o2)
   -0.25000000) T2(o1,o2,o3,a) V2(c1,c2,c3,c4) E5(c1,c2,i,k,o3,c3,c4,m,o2,o1)
   -0.25000000) T2(o1,o2,m,a) V2(c1,c2,c3,c4) E4(c1,c2,i,k,c3,c4,o1,o2)
   -0.25000000) T2(o1,o2,o3,a) V2(c1,c2,c3,c4) E5(c1,c2,m,o1,o2,c3,c4,i,o3,k)
   -0.25000000) \ \ T2(o1,o2,m,a) \ \ V2(c1,c2,c3,c4) \ \ E4(c1,c2,o1,o2,c3,c4,i,k)
    0.25000000) T2(01,02,03,a) V2(c1,c2,c3,c4) E5(c1,c2,m,o1,o2,c3,c4,i,o3,k)
    0.25000000) T2(o1,o2,m,a) V2(c1,c2,c3,c4) E4(c1,c2,o1,o2,c3,c4,i,k)
    0.25000000) T2(o1,o2,o3,a) V2(c1,o4,c2,o5) E5(c1,i,k,o3,o4,c2,m,o2,o1,o5)
    0.25000000) T2(o1,o2,m,a) V2(c1,o3,c2,o4) E4(c1,i,k,o3,c2,o1,o2,o4)
    0.25000000) T2(o1,o2,o3,a) V2(c1,m,c2,o4) E4(c1,i,k,o3,c2,o4,o2,o1)
      \hbox{\tt 0.25000000)} \ \hbox{\tt T2(ol,o2,o3,a)} \ \hbox{\tt V2(cl,o3,c2,o4)} \ \hbox{\tt E4(cl,i,k,o4,c2,m,o2,o1)} 
     0.25000000) T2(o1,o2,o3,a) V2(c1,m,c2,o3) E3(c1,i,k,c2,o1,o2)
   -0.25000000) T2(01,02,03,a) V2(c1,04,c2,05) E5(c1,i,k,03,04,c2,m,02,01,05)
   -0.25000000) T2(o1,o2,m,a) V2(c1,o3,c2,o4) E4(c1,i,k,o3,c2,o1,o2,o4)
   -0.25000000) T2(o1,o2,o3,a) V2(c1,m,c2,o4) E4(c1,i,k,o3,c2,o4,o2,o1)
   -0.25000000) T2(01,02,03,a) V2(c1,01,c2,04) E4(c1,i,k,03,c2,m,02,04)
   -0.25000000) T2(o1,o2,m,a) V2(c1,o1,c2,o3) E3(c1,i,k,c2,o3,o2)
   -0.25000000) T2(01,02,03,a) V2(c1,02,c2,04) E4(c1,i,k,03,c2,m,04,01)
   -0.25000000) T2(o1,o2,m,a) V2(c1,o2,c2,o3) E3(c1,i,k,c2,o1,o3)
   -0.25000000) T2(01,02,03,a) V2(c1,04,c2,05) E5(c1,m,01,02,04,c2,i,03,k,05)
   -0.25000000) T2(o1,o2,m,a) V2(c1,o3,c2,o4) E4(c1,o1,o2,o3,c2,i,k,o4)
   -0.25000000) T2(o1,o2,o3,a) V2(c1,o3,c2,o4) E4(c1,m,o1,o2,c2,i,o4,k)
   -0.25000000) T2(01,02,03,a) V2(c1,i,c2,04) E4(c1,m,01,02,c2,04,03,k)
   -0.25000000) T2(o1,o2,m,a) V2(c1,i,c2,o3) E3(c1,o1,o2,c2,o3,k)
   -0.25000000) T2(01,02,03,a) V2(c1,k,c2,04) E4(c1,m,01,02,c2,i,03,04)
   -0.25000000) T2(o1,o2,m,a) V2(c1,k,c2,o3) E3(c1,o1,o2,c2,i,o3)
    0.25000000) T2(o1,o2,o3,a) V2(c1,o4,c2,o5) E5(c1,m,o1,o2,o4,c2,i,o3,k,o5)
    0.25000000) T2(o1,o2,m,a) V2(c1,o3,c2,o4) E4(c1,o1,o2,o3,c2,i,k,o4)
    0.25000000) T2(o1,o2,o3,a) V2(c1,o3,c2,o4) E4(c1,m,o1,o2,c2,i,o4,k)
    0.25000000) T2(01,02,03,a) V2(c1,m,c2,04) E4(c1,01,02,04,c2,03,k,i)
    0.25000000) T2(o1,o2,o3,a) V2(c1,m,c2,o3) E3(c1,o1,o2,c2,i,k)
     0.25000000) T2(01,02,03,a) V2(c1,c2,05,04) E5(c1,i,k,03,04,05,m,02,01,c2)
    0.25000000) T2(o1,o2,m,a) V2(c1,c2,o4,o3) E4(c1,i,k,o3,o4,o1,o2,c2)
    0.25000000) T2(o1,o2,o3,a) V2(c1,c2,o4,m) E4(c1,i,k,o3,o4,c2,o2,o1)
     0.25000000) T2(01,02,03,a) V2(c1,c2,03,04) E4(c1,i,k,04,01,m,02,c2)
     0.25000000) T2(o1,o2,o3,a) V2(c1,c2,o3,m) E3(c1,i,k,o1,c2,o2)
   -0.25000000) T2(o1,o2,o3,a) V2(c1,c2,o5,o4) E5(c1,i,k,o3,o4,o5,m,o2,o1,c2)
   -0.25000000) T2(o1,o2,m,a) V2(c1,c2,o4,o3) E4(c1,i,k,o3,o4,o1,o2,c2)
   -0.25000000) T2(o1,o2,o3,a) V2(c1,c2,o4,m) E4(c1,i,k,o3,o4,c2,o2,o1)
   -0.25000000) T2(o1,o2,o3,a) V2(c1,c2,o4,o1) E4(c1,i,k,o3,o4,m,o2,c2)
   -0.25000000) T2(o1,o2,m,a) V2(c1,c2,o3,o1) E3(c1,i,k,o3,c2,o2)
   -0.25000000) T2(01,02,03,a) V2(c1,c2,04,02) E4(c1,i,k,03,04,m,c2,01)
   -0.25000000) T2(o1,o2,m,a) V2(c1,c2,o3,o2) E3(c1,i,k,o3,o1,c2)
   -0.25000000) \ \ T2(o1,o2,o3,a) \ \ V2(c1,c2,o5,o4) \ \ E5(c1,m,o1,o2,o4,o5,i,o3,k,c2)
   -0.25000000) T2(o1,o2,m,a) V2(c1,c2,o4,o3) E4(c1,o1,o2,o3,o4,i,k,c2)
   -0.25000000) \ \ T2(o1,o2,o3,a) \ \ V2(c1,c2,o4,o3) \ \ E4(c1,m,o1,o2,o4,i,c2,k)
   -0.25000000) T2(o1,o2,o3,a) V2(c1,c2,o4,i) E4(c1,m,o1,o2,o4,c2,o3,k)
   -0.25000000) T2(o1,o2,m,a) V2(c1,c2,o3,i) E3(c1,o1,o2,o3,c2,k)
   -0.25000000) T2(o1,o2,o3,a) V2(c1,c2,o4,k) E4(c1,m,o1,o2,o4,i,o3,c2)
```

9 11, 12 16:46	eclipse_sort.dat	Page 94/145
	T2(o1,o2,m,a) V2(c1,c2,o3,k) E3(c1,o1,o2,o3,i,c2)	
	T2(01,02,03,a) V2(c1,c2,05,04) E5(c1,m,01,02,04,c	
	T2(o1,o2,m,a) V2(c1,c2,o4,o3) E4(c1,o1,o2,o3,o4,i	
	T2(o1,o2,o3,a) V2(c1,c2,o4,o3) E4(c1,m,o1,o2,o4,i	
	T2(01,02,03,a) V2(c1,c2,m,o4) E4(c1,o1,o2,o4,i,o3 T2(o1,o2,o3,a) V2(c1,c2,m,o3) E3(c1,o1,o2,i,c2,k)	
	T2(01,02,03,a) $V2(c1,c2,m,03)$ $E3(c1,01,02,1,c2,k)T2(01,02,03,v1)$ $V2(c1,a,c2,v1)$ $E4(c1,i,k,03,c2,m,$	
	T2(01,02,03,V1) V2(c1,a,c2,V1) E4(c1,1,k,c3,c2,m, T2(01,02,m,V1) V2(c1,a,c2,V1) E3(c1,1,k,c2,01,02)	
	T2(01,02,03,v1) V2(c1,a,c2,v1) E4(c1,m,o1,o2,c2,i	
	T2(o1,o2,m,v1) $V2(c1,a,c2,v1)$ $E3(c1,o1,o2,c2,i,k)$	
	T2(01,02,03,v1) V2(c1,c2,v1,a) E4(c1,i,k,03,02,m,	
	T2(o1,o2,m,v1) $V2(c1,c2,v1,a)$ $E3(c1,i,k,o2,o1,c2)$	
	T2(o1,o2,o3,v1) $V2(c1,c2,a,v1)$ $E4(c1,m,o1,o2,k,i,v2,v3,v3,v3,v3,v3,v3,v3,v3,v3,v3,v3,v3,v3,$	
	T2(o1,o2,m,v1) V2(c1,c2,a,v1) E3(c1,o1,o2,k,i,c2)	
	T2(o1,o2,o3,a) V2(c1,c2,o5,o4) E5(c1,i,k,o3,o4,o5	
	T2(o1,o2,m,a) V2(c1,c2,o4,o3) E4(c1,i,k,o3,o4,o1,	
	T2(01,02,03,a) V2(c1,c2,04,m) E4(c1,i,k,03,04,c2,	
	T2(01,02,03,a) $V2(c1,c2,03,04)$ $E4(c1,i,k,04,01,m,$ $T2(01,02,03,a)$ $V2(c1,c2,03,m)$ $E3(c1,i,k,01,c2,02)$	
	T2(01,02,03,a) V2(c1,c2,05,04) E5(c1,i,k,03,04,05	
	T2(01,02,m,a) $V2(c1,c2,o4,o3)$ $E4(c1,i,k,o3,o4,o1,o3)$	
	T2(01,02,03,a) V2(c1,c2,04,m) E4(c1,i,k,03,04,c2,	
(-0.2500000)	T2(o1,o2,o3,a) $V2(c1,c2,o4,o1)$ $E4(c1,i,k,o3,o4,m,$	o2,c2)
	T2(o1,o2,m,a) V2(c1,c2,o3,o1) E3(c1,i,k,o3,c2,o2)	
	T2(01,02,03,a) V2(c1,c2,04,02) E4(c1,i,k,03,04,m,	
	T2(o1,o2,m,a) V2(c1,c2,o3,o2) E3(c1,i,k,o3,o1,c2)	
	T2(01,02,03,a) V2(c1,c2,05,04) E5(c1,m,01,02,04,c	
	T2(o1,o2,m,a) V2(c1,c2,o4,o3) E4(c1,o1,o2,o3,o4,i	
	T2(01,02,03,a) V2(c1,c2,04,03) E4(c1,m,01,02,04,i T2(01,02,03,a) V2(c1,c2,04,i) E4(c1,m,01,02,04,c2	
	T2(01,02,03,d) V2(c1,c2,03,i) E3(c1,01,02,03,c2,k)	
	T2(01,02,03,a) V2(c1,c2,04,k) E4(c1,m,01,02,04,i,	
	T2(o1,o2,m,a) $V2(c1,c2,o3,k)$ $E3(c1,o1,o2,o3,i,c2)$	
	T2(o1,o2,o3,a) V2(c1,c2,o5,o4) E5(c1,m,o1,o2,o4,c	
(0.2500000)	T2(o1,o2,m,a) V2(c1,c2,o4,o3) E4(c1,o1,o2,o3,o4,i	,k,c2)
	T2(o1,o2,o3,a) $V2(c1,c2,o4,o3)$ $E4(c1,m,o1,o2,o4,i3)$	
	T2(01,02,03,a) V2(c1,c2,m,04) E4(c1,01,02,04,i,03	
	T2(o1,o2,o3,a) V2(c1,c2,m,o3) E3(c1,o1,o2,i,c2,k)	
	T2(01,02,03,a) $V2(c1,04,c2,05)$ $E5(c1,i,k,03,04,c2)$ $T2(01,02,m,a)$ $V2(c1,03,c2,04)$ $E4(c1,i,k,03,c2,01,a)$	
	T2(01,02,03,a) V2(c1,03,c2,04) E4(c1,1,k,03,c2,01, T2(01,02,03,a) V2(c1,m,c2,04) E4(c1,i,k,03,c2,04,	
	T2(01,02,03,a) V2(c1,03,c2,04) E4(c1,i,k,04,c2,m,	
	T2(01,02,03,a) V2(c1,m,c2,03) E3(c1,i,k,c2,01,02)	
	T2(01,02,03,a) V2(c1,04,c2,05) E5(c1,i,k,03,04,c2	
	T2(o1,o2,m,a) V2(c1,o3,c2,o4) E4(c1,i,k,o3,c2,o1,	
	T2(o1,o2,o3,a) $V2(c1,m,c2,o4)$ $E4(c1,i,k,o3,c2,o4,$	
	T2(01,02,03,a) V2(c1,01,c2,04) E4(c1,i,k,03,c2,m,	
	T2(o1,o2,m,a) V2(c1,o1,c2,o3) E3(c1,i,k,c2,o3,o2)	
	T2(01,02,03,a) $V2(c1,02,c2,04)$ $E4(c1,i,k,03,c2,m,$	
	T2(01,02,m,a) V2(c1,02,c2,03) E3(c1,i,k,c2,01,03) T2(01,02,03,a) V2(c1,04,c2,05) E5(c1,m,01,02,04,c	
	T2(01,02,03,d) V2(c1,04,c2,03) E3(c1,m,01,02,04,c T2(01,02,m,a) V2(c1,03,c2,04) E4(c1,01,02,03,c2,i	
	T2(01,02,03,a) V2(c1,03,c2,04) E4(c1,m,01,02,c2,i	
	T2(o1,o2,o3,a) V2(c1,i,c2,o4) E4(c1,m,o1,o2,c2,o4	
(-0.25000000)	T2(o1,o2,m,a) $V2(c1,i,c2,o3)$ $E3(c1,o1,o2,c2,o3,k)$	
(-0.25000000)	T2(o1,o2,o3,a) $V2(c1,k,c2,o4)$ $E4(c1,m,o1,o2,c2,i,$	03,04)
(-0.25000000)	T2(o1,o2,m,a) $V2(c1,k,c2,o3)$ $E3(c1,o1,o2,c2,i,o3)$	
	T2(01,02,03,a) V2(c1,04,c2,05) E5(c1,m,01,02,04,c	
	T2(o1,o2,m,a) V2(c1,o3,c2,o4) E4(c1,o1,o2,o3,c2,i	
	T2(o1,o2,o3,a) V2(c1,o3,c2,o4) E4(c1,m,o1,o2,c2,i	
	T2(01,02,03,a) $V2(c1,m,c2,04)$ $E4(c1,01,02,04,c2,c3)$ $T2(01,02,03,a)$ $V2(c1,m,c2,03)$ $E3(c1,01,02,c2,i,k)$	
	T2(01,02,03,a) V2(01,m,02,03) E3(01,01,02,02,1,k) T2(01,02,03,a) V2(04,05,06,07) E5(1,k,03,04,05,m,	
(0.25000000)	T2(01,02,03,a) V2(04,05,06,07) E3(1,k,03,04,05,m, T2(01,02,m,a) V2(03,04,05,06) E4(1,k,03,04,01,02,	05.06)
(0.25000000)	T2(01,02,m,a) V2(03,04,05,06) E4(1,k,03,04,05,02, T2(01,02,03,a) V2(m,04,05,06) E4(1,k,03,04,05,02,	01,06)
	T2(01,02,03,a) V2(m,04,06,05) E4(i,k,03,04,06,02,	
	T2(01,02,03,a) V2(03,05,04,06) E4(i,k,04,05,m,02,	
	T2(o1,o2,o3,a) V2(m,o4,o3,o5) E3(i,k,o4,o1,o2,o5)	
(0.25000000)	T2(o1,o2,o3,a) V2(m,o3,o5,o4) E3(i,k,o4,o5,o2,o1)	

9 11, 12 16:46	eclipse_sort.dat	Page 95/145
(0.25000000)	T2(o1,o2,o3,a) V2(o3,o4,o5,o6) E4(i,k,o4,o5,m,o2	,06,01)
	T2(01,02,03,a) V2(m,03,05,04) E3(i,k,04,05,02,01	
	T2(01,02,03,a) V2(m,04,03,05) E3(i,k,04,01,02,05 T2(01,02,03,a) V2(04,05,06,07) E5(i,k,03,04,05,m	
	T2(01,02,m,a) V2(03,04,05,06) E4(i,k,03,04,01,02	
	T2(01,02,03,a) $V2(m,04,05,06)$ $E4(i,k,03,04,05,02)$	
	T2(01,02,03,a) V2(m,04,06,05) E4(i,k,03,04,06,02 T2(01,02,03,a) V2(01,04,05,06) E4(i,k,03,04,m,02	
	T2(01,02,m,a) V2(01,03,04,05) E3(i,k,03,04,02,05	
(-0.25000000)	T2(o1,o2,o3,a) V2(m,o1,o5,o4) E3(i,k,o3,o5,o2,o4)
	T2(01,02,03,a) V2(01,04,06,05) E4(i,k,03,04,m,02	
	T2(01,02,m,a) V2(01,03,05,04) E3(i,k,03,05,02,04 T2(01,02,03,a) V2(m,01,04,05) E3(i,k,03,04,02,05	
	T2(01,02,03,a) V2(02,04,05,06) E4(i,k,03,04,m,05	
	T2(o1,o2,m,a) V2(o2,o3,o4,o5) E3(i,k,o3,o1,o4,o5	
	T2(01,02,03,a) V2(m,02,05,04) E3(i,k,03,05,04,01	
	T2(01,02,03,a) V2(02,04,06,05) E4(i,k,03,04,m,06 T2(01,02,m,a) V2(02,03,05,04) E3(i,k,03,01,05,04	
	T2(01,02,03,a) $V2(m,02,04,05)$ $E3(i,k,03,04,05,01)$	
	T2(01,02,03,a) $V2(01,02,04,05)$ $E3(i,k,03,m,05,04)$)
	T2(01,02,m,a) $V2(01,02,03,04)$ $E2(i,k,03,04)$	\
	T2(01,02,03,a) $V2(01,02,05,04)$ $E3(i,k,03,m,04,05)$ $T2(01,02,m,a)$ $V2(01,02,04,03)$ $E2(i,k,04,03)$,
	T2(01,02,03,a) $V2(04,05,06,07)$ $E5(m,01,02,04,05,a)$	i,o3,k,o6,o7)
	T2(01,02,m,a) V2(03,04,05,06) E4(01,02,03,04,i,k	
	T2(01,02,03,a) V2(03,04,05,06) E4(m,01,02,04,i,o T2(01,02,03,a) V2(03,04,06,05) E4(m,01,02,04,i,o	
	T2(01,02,03,a) V2(03,04,00,03) E4(m,01,02,04,1,0	
	T2(o1,o2,m,a) V2(i,o3,o4,o5) E3(o1,o2,o3,o4,k,o5	
	T2(01,02,03,a) V2(i,03,04,05) E3(m,01,02,04,05,k	
	T2(01,02,03,a) $V2(i,04,06,05)$ $E4(m,01,02,04,06,0$ $T2(01,02,m,a)$ $V2(i,03,05,04)$ $E3(01,02,03,05,k,04)$	
	T2(01,02,03,a) V2(1,03,05,04) E3(m,01,02,05,04,k	
(-0.25000000)	T2(01,02,03,a) $V2(k,04,05,06)$ $E4(m,01,02,04,i,03)$,05,06)
	T2(01,02,m,a) $V2(k,03,04,05)$ $E3(01,02,03,i,04,05)$ $T2(01,02,03,a)$ $V2(k,03,04,05)$ $E3(m,01,02,i,05,04)$	
	T2(01,02,03,a) $V2(k,04,06,05)$ $E3(m,01,02,11,03,04)$ $T2(01,02,03,a)$ $V2(k,04,06,05)$ $E4(m,01,02,04,i,03)$	
(-0.25000000)	T2(o1,o2,m,a) $V2(k,o3,o5,o4)$ $E3(o1,o2,o3,i,o5,o4)$)
	T2(01,02,03,a) V2(k,03,05,04) E3(m,01,02,i,04,05	
	T2(01,02,03,a) V2(i,k,04,05) E3(m,01,02,04,03,05 T2(01,02,m,a) V2(i,k,03,04) E2(01,02,03,04))
	T2(01,02,03,a) V2(i,k,05,04) E3(m,01,02,05,03,04)
(-0.25000000)	T2(o1,o2,m,a) $V2(i,k,o4,o3)$ $E2(o1,o2,o4,o3)$	
	T2(01,02,03,a) $V2(04,05,06,07)$ $E5(m,01,02,04,05,07)$	
	T2(01,02,m,a) $V2(03,04,05,06)$ $E4(01,02,03,04,i,k)$ $T2(01,02,03,a)$ $V2(03,04,05,06)$ $E4(m,01,02,04,i,0)$	
	T2(01,02,03,a) V2(03,04,06,05) E4(m,01,02,04,i,0	
	T2(01,02,03,a) V2(m,05,04,06) E4(01,02,04,05,03,	
	T2(01,02,03,a) V2(m,04,03,05) E3(01,02,04,i,k,05 T2(01,02,03,a) V2(m,03,04,05) E3(01,02,04,05,k,i	
	T2(01,02,03,a) $V2(m,04,05,06)$ $E4(01,02,04,05,03,13)$	
	T2(o1,o2,o3,a) V2(m,o3,o4,o5) E3(o1,o2,o4,o5,k,i	
	T2(01,02,03,a) V2(m,04,03,05) E3(01,02,04,i,k,05	
	T2(01,02,03,v1) $V2(04,a,05,v1)$ $E4(i,k,03,04,m,02)$ $T2(01,02,m,v1)$ $V2(03,a,04,v1)$ $E3(i,k,03,01,02,04)$	
	T2(o1,o2,o3,v1) V2(m,a,o4,v1) E3(i,k,o3,o4,o2,o1	
	T2(01,02,03,v1) V2(03,a,04,v1) E3(i,k,04,m,02,01)
	T2(01,02,03,v1) $V2(m,a,03,v1)$ $E2(i,k,01,02)$ $T2(01,02,03,v1)$ $V2(04,a,05,v1)$ $E4(m,01,02,04,i,0)$	3 k o5)
	T2(01,02,03,V1) V2(04,a,03,V1) E4(m,01,02,04,1,0	
(0.25000000)	T2(01,02,03,v1) $V2(03,a,04,v1)$ $E3(m,01,02,i,04,k)$)
	T2(01,02,03,v1) $V2(m,a,04,v1)$ $E3(01,02,04,03,k,i)$)
	T2(01,02,03,v1) $V2(m,a,03,v1)$ $E2(01,02,i,k)$ $T2(01,02,03,v1)$ $V2(04,05,v1,a)$ $E4(i,k,03,04,m,05)$,01,02)
(0.25000000)	T2(o1,o2,m,v1) $V2(o3,o4,v1,a)$ $E3(i,k,o3,o1,o4,o2)$)
	T2(01,02,03,v1) V2(m,04,v1,a) E3(i,k,03,02,04,01	
	T2(01,02,03,v1) V2(03,04,a,v1) E3(i,k,04,m,01,02 T2(01,02,03,v1) V2(m,03,v1,a) E2(i,k,02,01))
	T2(01,02,03,V1) $V2(m,03,V1,d)$ $E2(1,K,02,01)$ $T2(01,02,03,V1)$ $V2(04,05,a,V1)$ $E4(m,01,02,04,i,0)$	3,o5,k)

9 11, 12 16:46	eclipse_sort.dat	Page 06/1/15
	T2(01,02,m,v1) V2(03,04,a,v1) E3(01,02,03,i,04,k)	Page 96/145
(0.25000000) (0.25000000)	T2(01,02,m,V1) V2(03,04,a,V1) E3(01,02,03,1,4,4) T2(01,02,03,V1) V2(m,04,V1,a) E3(01,02,04,03,i,k) T2(01,02,03,V1) V2(m,03,V1,a) E2(01,02,k,i) T2(01,02,03,V1) V2(c1,c2,V1,a) E4(c1,i,k,03,02,m, T2(01,02,03,V1) V2(c1,c2,V1,a) E3(c1,i,k,02,01,c2) T2(01,02,03,V1) V2(c1,c2,a,V1) E4(c1,i,k,03,c2,m, T2(01,02,m,V1) V2(c1,c2,a,V1) E3(c1,01,02,k,i,c2) T2(01,02,m,V1) V2(c1,a,c2,V1) E3(c1,01,02,k,i,c2) T2(01,02,m,V1) V2(c1,a,c2,V1) E3(c1,i,k,c2,01,02) T2(01,02,03,V1) V2(c1,a,c2,V1) E3(c1,i,k,c2,01,02) T2(01,02,03,V1) V2(c1,a,c2,V1) E3(c1,i,k,03,02,m, T2(01,02,03,V1) V2(c1,a,c2,V1) E3(c1,01,02,c2,i,k) T2(01,02,03,V1) V2(c1,a,c2,V1) E3(c1,01,02,c2,i,k) T2(01,02,03,V1) V2(04,05,V1,a) E4(i,k,03,04,m,05, T2(01,02,03,V1) V2(m,04,V1,a) E3(i,k,03,01,04,02) T2(01,02,03,V1) V2(m,04,V1,a) E3(i,k,04,m,01,02) T2(01,02,03,V1) V2(m,04,V1,a) E3(i,k,04,m,01,02) T2(01,02,03,V1) V2(03,04,a,V1) E3(i,k,04,m,01,02) T2(01,02,03,V1) V2(03,04,a,V1) E3(01,02,04,i,03) T2(01,02,03,V1) V2(03,04,a,V1) E3(01,02,03,i,04,k) T2(01,02,03,V1) V2(03,04,a,V1) E3(01,02,03,i,04,k) T2(01,02,03,V1) V2(m,03,V1,a) E2(i,k,02,01) T2(01,02,03,V1) V2(m,04,V1,a) E3(01,02,04,03,i,k) T2(01,02,03,V1) V2(m,04,V1,a) E3(01,02,04,03,i,k) T2(01,02,03,V1) V2(m,04,V1) E3(i,k,03,01,02,04) T2(01,02,03,V1) V2(m,a,04,V1) E3(i,k,03,01,02,04) T2(01,02,03,V1) V2(m,a,04,V1) E3(i,k,03,01,02,04) T2(01,02,03,V1) V2(m,a,04,V1) E3(i,k,01,02) T2(01,02,03,V1) V2(m,a,04,V1) E3(i,k,01,02,04),03,i,k) T2(01,02,03,V1) V2(m,a,04,V1) E3(01,02,03,i,k,04) T2(01,02,03,V1) V2(m,a,04,V1) E3(01,02,03,i,k,04) T2(01,02,03,V1) V2(m,a,04,V1) E3(01,02,04,03,i,k) T2(01,02,03,V1) V2(m,a,03,V1) E3(01,02,04,03,i,k)	(c2,o1) (o3,c2) (o2,o1) (o2,o1) (o1,o2) (o1,o2) (o1,o5)
1 : (0.5 2 : (1.0 3 : (-0.5 4 : (-0.5 5 : (-0.5 6 : (-0.5 7 : (-0.5 8 : (-0.5 10 : (-0.5 11 : (1.0 12 : (1.0 13 : (1.0 14 : (1.0 15 : (2.0 16 : (-1.0 17 : (-1.0 18 : (-1.0 19 : (-1.0 20 : (-1.0 21 : (-1.0 22 : (-1.0 23 : (-0.5 25 : (-0.5 26 : (-0.5 27 : (0.5 28 : (0.5	0000000) D3(i,k,o4,o3,o2,o1) T2(o1,o2,o4,a) h(m,o2,000000) D3(i,k,o4,m,o3,o2) T2(o2,o3,o1,a) h(o4,o1,000000) D3(i,k,o4,m,o3,o2) T2(o3,o2,o1,a) h(m,o1) 000000) D3(i,k,o4,m,o3,o2) T2(o1,o3,o4,a) h(o2,o1,000000) D3(i,k,o4,m,o3,o2) T2(o1,o2,m,a) h(o3,o1) 000000) D3(i,k,o4,m,o3,o2) T2(o1,o2,m,a) h(o3,o1) 000000) D3(i,k,o4,m,o3,o2) T2(o2,o1,o4,a) h(o3,o1,o1,o1,o1,o1,o1,o1,o1,o1,o1,o1,o1,o1,	m,cl,o3) 4,cl,o1) 1) 2,cl,o1) 1) 2,cl,o1) 1) 2,cl,o1) 1) 2,cl,o1) 1) 2,cl,o3) 3,cl,o4) 1,cl,o3) 3,cl,o4) 2,cl,o3) 3,cl,o4) 1,cl,o3) 3,cl,o4,o1) 1,cl,o3) 1,cl,o3,o3) 1,cl,o4,o1) 1,cl,o2,o1) 1,cl,o2,o1) 1,cl,o2,o1)

9 11, 12 16:46	eclipse_sort.dat	Page 97/145
31 : (0.50000000) 32 : (0.50000000) 33 : (0.50000000) 34 : (0.50000000) 35 : (2.00000000) 36 : (2.00000000) 37 : (-1.00000000) 38 : (-1.00000000)	D2(i,k,o3,o2) T2(o3,o1,m,a) V2(c1,c) D3(k,o4,o3,o2,o1,m) T2(o1,o2,o4,a) D2(k,o3,o2,o1) T2(o1,o2,m,a) V2(c1,c) D3(i,o4,o3,m,o2,o1) T2(o2,o1,o4,a) D2(i,o3,o2,o1) T2(o2,o1,m,a) V2(c1,c) D3(i,k,o3,m,o2,o1) T2(o1,o2,o3,v1) D2(i,k,o2,o1) T2(o2,o1,m,v1) V2(c1,c) D3(i,k,o3,m,o2,o1) T2(o1,o2,o3,v1) D2(i,k,o2,o1) T2(o2,o1,m,v1) V2(c1,c) D3(i,k,o3,m,o2,o1) T2(o1,o2,o3,v1) D2(i,k,o2,o1) T2(o2,o1,m,v1) V2(c1,c) D4(i,k,o6,o5,o4,o3,o2,o1) T2(o2,o3,o3,o2,o1) T2(o2,o3,o3,o2,o2,o1) T2(o2,o3,o3,o2,o2,o1) T2(o2,o3,o3,o2,o2,o1) T2(o2,o3,o3,o2,o2,o1) T2(o2,o3,o3,o2,o2,o2,o2,o2,o2,o2,o2,o2,o2,o2,o2,o2,	V2(c1,c1,i,o3) c1,i,o3) V2(c1,c1,k,o3) c1,k,o3) V2(c1,a,c1,v1) a,c1,v1) V2(c1,c1,a,v1) c1,a,v1)
41 : (1.00000000) 42 : (1.00000000)	D4(i,k,o6,o5,m,o4,o3,o2) T2(o3,o4,o D3(i,k,o5,o4,o3,o2) T2(o4,o3,o1,a) D3(i,k,o5,o4,o3,o2) T2(o2,o3,o1,a) D4(i,k,o6,o5,m,o4,o3,o2) T2(o1,o4,o	V2(m,o5,o1,o2) V2(m,o5,o4,o1)
44 : (-0.50000000) 45 : (-0.50000000) 46 : (-0.50000000)	D3(i,k,o5,o4,o3,o2) T2(o1,o3,m,a) V D3(i,k,o5,o4,o3,o2) T2(o1,o3,o5,a) D4(i,k,o6,o5,m,o4,o3,o2) T2(o3,o1,o	V2(05,04,02,01) V2(m,02,04,01) 6,a) V2(05,04,02,01)
48 : (-0.50000000) 49 : (-0.50000000) 50 : (-0.50000000)	D3(i,k,o5,o4,o3,o2) T2(o4,o1,m,a) V D3(i,k,o5,o4,o3,o2) T2(o2,o1,o5,a) V D3(i,k,o5,m,o4,o3) T2(o2,o1,o5,a) V D2(i,k,o4,o3) T2(o2,o1,m,a) V2(o4,o D4(k,o6,o5,o4,o3,o2,m,o1) T2(o2,o3,	V2(m, 03, 04, 01) 2(04, 03, 01, 02) 3, 02, 01)
53 : (-0.50000000)	$\begin{array}{lll} \text{D3}(k,05,04,03,02,01) & \text{T2}(02,03,\text{m,a}) \\ \text{D3}(k,05,04,03,\text{m,o2}) & \text{T2}(02,03,01,\text{a}) \\ \text{D4}(i,06,05,04,\text{m,o3},02,01) & \text{T2}(03,02,01) \end{array}$	V2(i,o4,o5,o1)
56 : (-0.50000000) 57 : (-0.50000000) 58 : (-0.50000000)	D3(i,o5,o4,o3,o2,o1) T2(o3,o2,m,a) D3(i,o5,o4,m,o3,o2) T2(o2,o3,o1,a) D3(m,o5,o4,o3,o2,o1) T2(o5,o4,o2,a) D2(o4,o3,o2,o1) T2(o4,o3,m,a) V2(i, D4(i,k,o1,o2,m,o3,o4,o5) T2(o4,o3,o	V2(k,o4,o5,o1) V2(i,k,o3,o1) k,o2,o1)
61 : (1.00000000) 62 : (1.00000000) 63 : (1.00000000)	D3(i,k,o4,o3,o2,o1) T2(o3,o2,m,v1) D3(i,k,o1,o2,o3,o4) T2(o4,o3,o1,v1) D3(i,k,o1,m,o2,o3) T2(o3,o2,o4,v1) D2(i,k,o1,o2) T2(o1,o2,o3,v1) V2(m, D4(i,k,o1,o2,m,o3,o4,o5) T2(o4,o5,o	V2(m,a,o2,v1) V2(o1,a,o4,v1) a,o3,v1)
66: (1.00000000) 67: (1.00000000) 68: (1.00000000) 69: (1.00000000)	D3(i,k,o4,o3,o2,o1) T2(o3,o1,m,v1) D3(i,k,o1,o2,o3,o4) T2(o4,o2,o1,v1) D3(i,k,o1,m,o2,o3) T2(o2,o3,o4,v1) D2(i,k,o1,o2) T2(o2,o1,o3,v1) V2(m, Ecas D3(i,k,o1,m,o2,o3) T2(o3,o2,o1 Ecas D2(i,k,o1,m,o2,o3) T2(o3,o2,o1	V2(m,o3,v1,a) V2(o1,o4,v1,a) o3,v1,a)
1 : (0.50000000) 2 : (1.00000000) 3 : (-0.50000000) 4 : (-0.50000000) 6 : (-0.50000000) 7 : (-0.50000000) 8 : (-0.50000000) 9 : (-0.50000000) 10 : (-0.50000000) 11 : (1.0000000) 12 : (1.00000000) 13 : (1.00000000) 15 : (2.00000000)	D3(i,o3,k,o2,o4,o1) T2(o1,o2,o4,a) D3(i,m,k,o3,o4,o2) T2(o2,o3,o1,a) h D2(i,o3,k,o2) T2(o3,o2,o1,a) h(m,o1) D3(i,m,k,o3,o4,o2) T2(o1,o3,o4,a) h D2(i,o3,k,o2) T2(o1,o2,m,a) h(o3,o1) D3(i,m,k,o3,o4,o2) T2(o2,o1,o4,a) h D2(i,o3,k,o2) T2(o3,o1,m,a) h(o2,o1) D3(i,o4,o1,m,o2,o3) T2(o3,o4,o2,a) D2(i,o3,o1,o2) T2(o2,o1,o4,a) h D3(i,m,o3,o1,o4,o2) T2(o2,o1,o4,a) D2(i,o2,o3,o1) T2(o2,o1,m,a) h(k,o3) D3(i,m,k,o2,o1,o3) T2(o3,o2,o1,v1) D2(i,o1,k,o2) T2(o1,o2,m,v1) h(a,v1) D3(i,m,k,o3,o4,o2) T2(o2,o3,o1,a) V D3(i,m,k,o3,o4,o2) T2(o2,o3,o1,a) V D2(i,o3,k,o2) T2(o3,o2,o1,a) V D2(i,o3,k,o2) T2(o3,o2,o1,a) V D2(i,o3,k,o2) T2(o3,o2,o1,a) V D2(i,o3,k,o2) T2(o3,o2,o1,a) V	(04,01)) (02,01)) (03,01)) h(i,01)) h(k,03)) h(a,v1)) V2(c1,c1,m,03) '2(c1,c1,o1,o4) c1,m,01)

9 11, 12 16:46	eclipse_sort.dat	Page 98/145
·	D2(i,o3,k,o2) T2(o1,o2,m,a) V2(c1,c1,o1,	
18 : (-1.00000000)	D3(i,m,k,o3,o4,o2) T2(o2,o1,o4,a) V2(c1,	c1,o1,o3)
	D2(i,o3,k,o2) T2(o3,o1,m,a) V2(c1,c1,o1, D3(k,o2,o3,m,o4,o1) T2(o1,o2,o4,a) V2(c1	
21 : (-1.00000000)	D2(k,o2,o3,o1) $T2(o1,o2,m,a)$ $V2(c1,c1,i,a)$	03)
	D3(i,m,o3,o1,o4,o2) $T2(o2,o1,o4,a)$ $V2(c1)$ $D2(i,o2,o3,o1)$ $T2(o2,o1,m,a)$ $V2(c1,c1,k,a)$	
	D3(i,o3,k,o2,o4,o1) T2(o1,o2,o4,a) V2(c1	
	D3(i,m,k,o3,o4,o2) T2(o2,o3,o1,a) V2(c1,	
	D2(i,o3,k,o2) T2(o3,o2,o1,a) V2(c1,m,c1, D3(i,m,k,o3,o4,o2) T2(o1,o3,o4,a) V2(c1,	
28 : (0.50000000)	D2(i,o3,k,o2) $T2(o1,o2,m,a)$ $V2(c1,o1,c1,$	03)
	D3(i,m,k,o3,o4,o2) T2(o2,o1,o4,a) V2(c1, D2(i,o3,k,o2) T2(o3,o1,m,a) V2(c1,o1,c1,	
31 : (0.50000000)	D3(k,o2,o3,m,o4,o1) T2(o1,o2,o4,a) V2(c1	,i,c1,o3)
	D2(k,o2,o3,o1) $T2(o1,o2,m,a)$ $V2(c1,i,c1,$	
	D3(i,m,o3,o1,o4,o2) $T2(o2,o1,o4,a)$ $V2(c1)$ $D2(i,o2,o3,o1)$ $T2(o2,o1,m,a)$ $V2(c1,k,c1,a)$	
35 : (2.00000000)	D3(i,m,k,o2,o3,o1) T2(o1,o2,o3,v1) V2(c1	,c1,a,v1)
	D2(i,o2,k,o1) T2(o2,o1,m,v1) V2(c1,c1,a, D3(i,m,k,o2,o3,o1) T2(o1,o2,o3,v1) V2(c1	
38 : (-1.00000000)	D2(i,o2,k,o1) $T2(o2,o1,m,v1)$ $V2(c1,a,c1,$	v1)
39 : (0.50000000)	D4(i,o4,k,o3,o5,o1,o6,o2) T2(o2,o3,o6,a)	V2(m,o4,o1,o5)
40 : (0.5000000)	D4(i,m,k,o4,o5,o2,o6,o3) T2(o3,o4,o1,a)	V2(o1,o6,o2,o5)
41 : (1.00000000)	D3(i,o4,k,o3,o5,o2) T2(o4,o3,o1,a) V2(m,	01,02,05)
	D3(i,o4,k,o3,o5,o2) T2(o2,o3,o1,a) V2(m,	
43 : (-0.50000000)	D4(i,m,k,o4,o5,o2,o6,o3) T2(o1,o4,o6,a)	VZ(01,03,02,05)
	D3(i,o4,k,o3,o5,o2) T2(o1,o3,m,a) V2(o1,	
	D3(i,o4,k,o3,o5,o2) T2(o1,o3,o5,a) V2(m, D4(i,m,k,o4,o5,o2,o6,o3) T2(o3,o1,o6,a)	
	D3(i,o4,k,o3,o5,o2) $T2(o4,o1,m,a)$ $V2(o1,D3(i,o4,k,o3,o5,o2)$ $T2(o2,o1,o5,a)$ $V2(m,o5,o4,k,o3,o5,o2)$	
	D3(i,m,k,o4,o5,o3) T2(o2,o1,o5,a) V2(o1,	
	D2(i,04,k,03) $T2(02,01,m,a)$ $V2(01,03,02,$	
31 . (-0.3000000)	D4(k,o3,o4,o1,o5,m,o6,o2) T2(o2,o3,o6,a)	V2(1,05,01,04)
	D3(k, 03, 04, 01, 05, 02) T2(02, 03, m, a) V2(i,	
	D3(k,o3,o4,o2,o5,m) T2(o2,o3,o1,a) V2(i, D4(i,m,o4,o1,o5,o2,o6,o3) T2(o3,o2,o6,a)	
	D3(i,o3,o4,o1,o5,o2) T2(o3,o2,m,a) V2(k, D3(i,m,o4,o2,o5,o3) T2(o2,o3,o1,a) V2(k,	
57 : (-0.50000000)	D3(m,o3,o4,o1,o5,o2) T2(o5,o4,o2,a) V2(i	,o3,k,o1)
	D2(01,03,02,04) T2(04,03,m,a) V2(i,02,k, D4(i,m,k,03,01,04,02,05) T2(04,03,01,v1)	
	B1(1,m,n,03,01,01,02,03) 12(01,03,01,V1)	VZ(0Z,03,0,VI)
	D3(i,o3,k,o2,o4,o1) T2(o3,o2,m,v1) V2(o1 D3(i,o2,k,o3,o1,o4) T2(o4,o3,o1,v1) V2(m	
	D3(i,m,k,o2,o1,o3) T2(o3,o2,o4,v1) V2(o1	
	D2(i,o1,k,o2) T2(o1,o2,o3,v1) V2(m,o3,a,	
64 : (1.00000000)	D4(i,m,k,o3,o1,o4,o2,o5) T2(o4,o5,o1,v1)	V2(02,v1,03,a)
	D3(i,o3,k,o2,o4,o1) T2(o3,o1,m,v1) V2(o2	
	D3(i,o2,k,o3,o1,o4) T2(o4,o2,o1,v1) V2(m D3(i,m,k,o2,o1,o3) T2(o2,o3,o4,v1) V2(o1	
68 : (1.00000000)	D2(i,o1,k,o2) T2(o2,o1,o3,v1) V2(m,v1,o3	
	Ecas D3(i,m,k,o2,o1,o3) T2(o3,o2,o1,a) Ecas D2(i,o1,k,o2) T2(o1,o2,m,a)	
, , , (1.00000000)	ECGS D2(1,01,K,02) 12(01,02,M,d)	
<pre>< RESULT > 0 : (0.50000000)</pre>	D3(i,o3,k,o2,o4,o1) T2(o1,o2,o4,a) h(m,o	(3)
1: (0.50000000)	D3(i,m,k,o3,o4,o2) T2(o2,o3,o1,a) h(o4,o	1)
2: (1.00000000)	D2(i,o3,k,o2) $T2(o3,o2,o1,a)$ $h(m,o1)$	
	D3(i,m,k,o3,o4,o2) $T2(o1,o3,o4,a)$ $h(o2,o2)$ $D2(i,o3,k,o2)$ $T2(o1,o2,m,a)$ $h(o3,o1)$) ±)

9 11, 12 16:46	eclipse_sort.dat	Page 99/145
	D3(i,m,k,o3,o4,o2) T2(o2,o1,o4,a) h(o	3,01)
	D2(i,o3,k,o2) $T2(o3,o1,m,a)$ $h(o2,o1)$ $D3(k,o4,o1,m,o2,o3)$ $T2(o3,o4,o2,a)$ $h(o2,o3)$	i.o1)
8 : (-0.50000000)	D2(k,o3,o1,o2) $T2(o2,o3,m,a)$ $h(i,o1)$	
	D3(i,m,o3,o1,o4,o2) $T2(o2,o1,o4,a)$ $h(l,o2)$	k, 03)
	D2(i,o2,o3,o1) T2(o2,o1,m,a) h(k,o3) D3(i,m,k,o2,o1,o3) T2(o3,o2,o1,v1) h(a	a,v1)
12: (1.00000000)	D2(i,o1,k,o2) $T2(o1,o2,m,v1)$ $h(a,v1)$	
	D3(i,o3,k,o2,o4,o1) T2(o1,o2,o4,a) V2 D3(i,m,k,o3,o4,o2) T2(o2,o3,o1,a) V2(o	
	D2(i,o3,k,o2) T2(o3,o2,o1,a) V2(c1,c1	
	D3(i,m,k,o3,o4,o2) T2(o1,o3,o4,a) V2(o1,o3,o4,a) V2(o1,o3,o4,a)	
	D2(i,o3,k,o2) T2(o1,o2,m,a) V2(c1,c1,c1,c3) D3(i,m,k,o3,o4,o2) T2(o2,o1,o4,a) V2(c1,c1,c2)	
19 : (-1.00000000)	D2(i,o3,k,o2) T2(o3,o1,m,a) V2(c1,c1,	01,02)
	D3(k,o2,o3,m,o4,o1) T2(o1,o2,o4,a) V2 D2(k,o2,o3,o1) T2(o1,o2,m,a) V2(c1,c1	
	D3(i,m,o3,o1,o4,o2) T2(o2,o1,o4,a) V2	
	D2(i,o2,o3,o1) T2(o2,o1,m,a) V2(c1,c1	
	D3(i,o3,k,o2,o4,o1) T2(o1,o2,o4,a) V2 D3(i,m,k,o3,o4,o2) T2(o2,o3,o1,a) V2(o	
26 : (-1.00000000)	D2(i,o3,k,o2) T2(o3,o2,o1,a) V2(c1,m,	c1,o1)
	D3(i,m,k,o3,o4,o2) T2(o1,o3,o4,a) V2(o2,o3,k,o2) T2(o1,o2,m,a) V2(c1,o1,o2,m,a) V2(c1,o1,o2,m,a) V2(c1,o1,o2,m,a) V2(c1,o1,o2,m,a) V2(c1,o1,o2,m,a) V2(c1,o1,o2,m,a) V2(c1,o1,o2,m,a) V2(c1,o2,m,a) V2	
	D3(i,m,k,o3,o4,o2) T2(o2,o1,o4,a) V2(c1,o1,o2,o1,o4,a) V2(c1,o1,o2,o1,o4,a)	
	D2(i,o3,k,o2) T2(o3,o1,m,a) V2(c1,o1,	
	D3(k,o2,o3,m,o4,o1) T2(o1,o2,o4,a) V2 D2(k,o2,o3,o1) T2(o1,o2,m,a) V2(c1,i,o2,o2,o3,o1)	
33 : (0.50000000)	D3(i,m,o3,o1,o4,o2) T2(o2,o1,o4,a) V2	(c1,k,c1,o3)
	D2(i,o2,o3,o1) T2(o2,o1,m,a) V2(c1,k,o3) (i,m,k,o2,o3,o1) T2(o1,o2,o3,v1) V2	
	D2(i,o2,k,o1) T2(o2,o1,m,v1) V2(c1,c1	
	D3(i,m,k,o2,o3,o1) T2(o1,o2,o3,v1) V2	
	D2(i,o2,k,o1) T2(o2,o1,m,v1) V2(c1,a,o4) D4(i,o4,k,o3,o5,o1,o6,o2) T2(o2,o3,o6)	
	D4(i,m,k,o4,o5,o2,o6,o3) T2(o3,o4,o1,	
	D3(i,o4,k,o3,o5,o2) T2(o4,o3,o1,a) V2	
42 : (1.00000000)	D3(i,o4,k,o3,o5,o2) T2(o2,o3,o1,a) V2	(m, o4, o1, o5)
43 : (-0.50000000)	D4(i,m,k,o4,o5,o2,o6,o3) T2(o1,o4,o6,	a) V2(o1,o3,o2,o5)
44 : (-0.50000000)	D3(i,o4,k,o3,o5,o2) T2(o1,o3,m,a) V2(01,04,02,05)
	D3(i, 04, k, 03, 05, 02) T2(01, 03, 05, a) V2	
40 . (-0.50000000)	D4(i,m,k,o4,o5,o2,o6,o3) T2(o3,o1,o6,	a) V2(01,04,02,03)
	D3(i,o4,k,o3,o5,o2) T2(o4,o1,m,a) V2(
	D3(i,o4,k,o3,o5,o2) T2(o2,o1,o5,a) V2 D3(i,m,k,o4,o5,o3) T2(o2,o1,o5,a) V2(o2,o1,o5,a) V2(o2,o1,o5,a)	
50 : (-0.50000000)	D2(i,o4,k,o3) T2(o2,o1,m,a) V2(o1,o3,	02,04)
51 : (-0.50000000)	D4(k,o3,o4,o1,o5,m,o6,o2) T2(o2,o3,o6	,a) V2(i,o5,o1,o4)
52 : (-0.50000000)	D3(k,o3,o4,o1,o5,o2) T2(o2,o3,m,a) V2	(i,o5,o1,o4)
	D3(k,o3,o4,o2,o5,m) T2(o2,o3,o1,a) V2	
54 : (-0.50000000)	D4(i,m,o4,o1,o5,o2,o6,o3) T2(o3,o2,o6	,a) V2(K,05,01,04)
	D3(i,o3,o4,o1,o5,o2) T2(o3,o2,m,a) V2	
56 : (-0.50000000) 57 : (-0.50000000)	D3(i,m,o4,o2,o5,o3) T2(o2,o3,o1,a) V2 D3(m,o3,o4,o1,o5,o2) T2(o5,o4,o2,a) V	(k,o5,o1,o4) 2(i o3 k o1)
58 : (-0.50000000)	D2(o1,o3,o2,o4) T2(o4,o3,m,a) V2(i,o2	,k,o1)
59 : (1.00000000)	D4(i,m,k,o3,o1,o4,o2,o5) T2(o4,o3,o1,	v1) V2(o2,o5,a,v1)
60: (1.00000000)	D3(i,o3,k,o2,o4,o1) T2(o3,o2,m,v1) V2	(o1,o4,a,v1)
61 : (1.00000000)	D3(i,o2,k,o3,o1,o4) T2(o4,o3,o1,v1) V	2(m,o2,a,v1)
	D3(i,m,k,o2,o1,o3) T2(o3,o2,o4,v1) V2 D2(i,o1,k,o2) T2(o1,o2,o3,v1) V2(m,o3	
	D4(i,m,k,o3,o1,o4,o2,o5) T2(o4,o5,o1,	
65 : (1.00000000)	D3(i,o3,k,o2,o4,o1) T2(o3,o1,m,v1) V2	(o2,a,o4,v1)

```
eclipse sort.dat
  9 11, 12 16:46
                                                                    Page 100/145
   66: (
             1.00000000) D3(i,o2,k,o3,o1,o4) T2(o4,o2,o1,v1) V2(m,v1,o3,a)
   67 :
             1.00000000) D3(i,m,k,o2,o1,o3) T2(o2,o3,o4,v1) V2(o1,v1,o4,a)
   68: (
             1.00000000) D2(i,o1,k,o2) T2(o2,o1,o3,v1) V2(m,v1,o3,a)
   69
      :
             1.00000000) Ecas D3(i,m,k,o2,o1,o3) T2(o3,o2,o1,a)
   70: (
             1.00000000) Ecas D2(i,o1,k,o2) T2(o1,o2,m,a)
Setting up parameters as default ....
! * 26 terms are replaced in the linking process
The linked formulas ....
         0.50000000) D3(i,o3,k,o2,o4,o1) T2(o1,o2,o4,a) h(m,o3)
         0.50000000) D3(i,m,k,o3,o4,o2) T2(o2,o3,o1,a) h(o4,o1)
2:
         1.00000000) D2(i,o3,k,o2) T2(o3,o2,o1,a) h(m,o1)
3 :
        -0.50000000) D3(i,m,k,o3,o4,o2) T2(o1,o3,o4,a) h(o2,o1)
        -0.50000000) D2(i,o3,k,o2) T2(o1,o2,m,a) h(o3,o1)
5:
        -0.50000000) D3(i,m,k,o3,o4,o2) T2(o2,o1,o4,a) h(o3,o1)
6:
        -0.50000000) D2(i,o3,k,o2) T2(o3,o1,m,a) h(o2,o1)
7 :
        -0.50000000) D3(k,o4,o1,m,o2,o3) T2(o3,o4,o2,a) h(i,o1)
8 :
        -0.50000000) D2(k,o3,o1,o2) T2(o2,o3,m,a) h(i,o1)
9: (
        -0.50000000) \ \ \text{D3(i,m,o3,o1,o4,o2)} \ \ \text{T2(o2,o1,o4,a)} \ \ \text{h(k,o3)}
         -0.50000000) D2(i,o2,o3,o1) T2(o2,o1,m,a) h(k,o3)
10 :
11 :
          1.00000000) D3(i,m,k,o2,o1,o3) T2(o3,o2,o1,v1) h(a,v1)
12 :
          1.00000000) D2(i,o1,k,o2) T2(o1,o2,m,v1) h(a,v1)
13:
          1.00000000) D3(i,o3,k,o2,o4,o1) T2(o1,o2,o4,a) Y0(m,o3)
14:
          1.00000000) D3(i,m,k,o3,o4,o2) T2(o2,o3,o1,a) Y1(o1,o4)
          2.00000000) D2(i,o3,k,o2) T2(o3,o2,o1,a) Y2(m,o1)
15 :
16:
         -1.00000000) D3(i,m,k,o3,o4,o2) T2(o1,o3,o4,a) Y3(o1,o2)
17: (
         -1.00000000) D2(i,o3,k,o2) T2(o1,o2,m,a) Y4(o1,o3)
18: (
         -1.00000000) D3(i,m,k,o3,o4,o2) T2(o2,o1,o4,a) Y5(o1,o3)
         -1.00000000) D2(i,o3,k,o2) T2(o3,o1,m,a) Y6(o1,o2)
19: (
20: (
         -1.00000000) D3(k,o2,o3,m,o4,o1) T2(o1,o2,o4,a) Y7(i,o3)
21 : (
         -1.00000000) D2(k,o2,o3,o1) T2(o1,o2,m,a) Y8(i,o3)
         -1.00000000) D3(i,m,o3,o1,o4,o2) T2(o2,o1,o4,a) Y9(k,o3)
23 : (
         -1.00000000) D2(i,o2,o3,o1) T2(o2,o1,m,a) Y10(k,o3)
24: (
         -0.50000000) D3(i,o3,k,o2,o4,o1) T2(o1,o2,o4,a) Y11(m,o3)
25 : (
         -0.50000000) D3(i,m,k,o3,o4,o2) T2(o2,o3,o1,a) Y12(o1,o4)
26: (
         -1.00000000) D2(i,o3,k,o2) T2(o3,o2,o1,a) Y13(m,o1)
27 : (
          0.50000000) D3(i,m,k,o3,o4,o2) T2(o1,o3,o4,a) Y14(o1,o2)
28: (
          0.50000000) D2(i,o3,k,o2) T2(o1,o2,m,a) Y15(o1,o3)
29: (
          0.50000000) D3(i,m,k,o3,o4,o2) T2(o2,o1,o4,a) Y16(o1,o3)
30: (
          0.50000000) D2(i,o3,k,o2) T2(o3,o1,m,a) Y17(o1,o2)
31: (
          0.50000000) D3(k,o2,o3,m,o4,o1) T2(o1,o2,o4,a) Y18(i,o3)
32: (
          0.50000000) D2(k,o2,o3,o1) T2(o1,o2,m,a) Y19(i,o3)
33 : (
          0.50000000) D3(i,m,o3,o1,o4,o2) T2(o2,o1,o4,a) Y20(k,o3)
          0.50000000) D2(i,o2,o3,o1) T2(o2,o1,m,a) Y21(k,o3)
35 : (
          2.00000000) D3(i,m,k,o2,o3,o1) T2(o1,o2,o3,v1) Y22(a,v1)
36 : (
          2.00000000) D2(i,o2,k,o1) T2(o2,o1,m,v1) Y23(a,v1)
37
         -1.00000000) D3(i,m,k,o2,o3,o1) T2(o1,o2,o3,v1) Y24(a,v1)
38
         -1.00000000) D2(i,o2,k,o1) T2(o2,o1,m,v1) Y25(a,v1)
39 : (
          0.50000000) D4(i,o4,k,o3,o5,o1,o6,o2) T2(o2,o3,o6,a) V2(m,o4,o1,o5)
40 : (
          0.50000000) D4(i,m,k,o4,o5,o2,o6,o3) T2(o3,o4,o1,a) V2(o1,o6,o2,o5)
41: (
          1.00000000) D3(i,o4,k,o3,o5,o2) T2(o4,o3,o1,a) V2(m,o1,o2,o5)
42: (
          1.00000000) D3(i,o4,k,o3,o5,o2) T2(o2,o3,o1,a) V2(m,o4,o1,o5)
43 : (
         -0.50000000) D4(i,m,k,o4,o5,o2,o6,o3) T2(o1,o4,o6,a) V2(o1,o3,o2,o5)
44
         -0.50000000) D3(i,o4,k,o3,o5,o2) T2(o1,o3,m,a) V2(o1,o4,o2,o5)
         -0.50000000) D3(i,o4,k,o3,o5,o2) T2(o1,o3,o5,a) V2(m,o4,o1,o2)
45
   : (
46 : (
         -0.50000000) D4(i,m,k,o4,o5,o2,o6,o3) T2(o3,o1,o6,a) V2(o1,o4,o2,o5)
47: (
         -0.50000000) D3(i,o4,k,o3,o5,o2) T2(o4,o1,m,a) V2(o1,o3,o2,o5)
48: (
         -0.50000000) D3(i,o4,k,o3,o5,o2) T2(o2,o1,o5,a) V2(m,o4,o1,o3)
```

```
eclipse_sort.dat
  9 11, 12 16:46
                                                                   Page 101/145
49: (
         -0.50000000) D3(i,m,k,o4,o5,o3) T2(o2,o1,o5,a) V2(o1,o4,o2,o3)
50: (
         -0.50000000) D2(i,o4,k,o3) T2(o2,o1,m,a) V2(o1,o3,o2,o4)
51 : (
52 : (
         -0.50000000) D4(k,o3,o4,o1,o5,m,o6,o2) T2(o2,o3,o6,a) V2(i,o5,o1,o4)
         -0.50000000) D3(k,o3,o4,o1,o5,o2) T2(o2,o3,m,a) V2(i,o5,o1,o4)
53 : (
        -0.50000000) D3(k,o3,o4,o2,o5,m) T2(o2,o3,o1,a) V2(i,o5,o1,o4)
        -0.50000000) D4(i,m,o4,o1,o5,o2,o6,o3) T2(o3,o2,o6,a) V2(k,o5,o1,o4)
55 : (
        -0.50000000) D3(i,o3,o4,o1,o5,o2) T2(o3,o2,m,a) V2(k,o5,o1,o4)
56: (
        -0.50000000) D3(i,m,o4,o2,o5,o3) T2(o2,o3,o1,a) V2(k,o5,o1,o4)
57 : (
        -0.50000000) D3(m,o3,o4,o1,o5,o2) T2(o5,o4,o2,a) V2(i,o3,k,o1)
58 : (
         -0.50000000) D2(o1,o3,o2,o4) T2(o4,o3,m,a) V2(i,o2,k,o1)
59: (
         1.00000000) D4(i,m,k,o3,o1,o4,o2,o5) T2(o4,o3,o1,v1) V2(o2,o5,a,v1)
60: (
         1.00000000) D3(i,o3,k,o2,o4,o1) T2(o3,o2,m,v1) V2(o1,o4,a,v1)
61: (
         1.00000000) D3(i,o2,k,o3,o1,o4) T2(o4,o3,o1,v1) V2(m,o2,a,v1)
         1.00000000) D3(i,m,k,o2,o1,o3) T2(o3,o2,o4,v1) V2(o1,o4,a,v1)
62: (
63: (
          1.00000000) D2(i,o1,k,o2) T2(o1,o2,o3,v1) V2(m,o3,a,v1)
64: (
          1.00000000) D4(i,m,k,o3,o1,o4,o2,o5) T2(o4,o5,o1,v1) V2(o2,v1,o3,a)
          1.000000000) D3(i,o3,k,o2,o4,o1) T2(o3,o1,m,v1) V2(o2,a,o4,v1)
65 : (
66 : (
         1.00000000) D3(i,o2,k,o3,o1,o4) T2(o4,o2,o1,v1) V2(m,v1,o3,a)
67 : (
          1.00000000) D3(i,m,k,o2,o1,o3) T2(o2,o3,o4,v1) V2(o1,v1,o4,a)
68 : (
          1.00000000) D2(i,o1,k,o2) T2(o2,o1,o3,v1) V2(m,v1,o3,a)
          1.00000000) Ecas D3(i,m,k,o2,o1,o3) T2(o3,o2,o1,a)
69 : (
70: (
          1.00000000) Ecas D2(i,o1,k,o2) T2(o1,o2,m,a)
The content of each effective tensor ....
Y0 < -- ( 1.00000000) V2(c1,c1,m,o3)
Y1 <-- (
          1.00000000) V2(c1,c1,o1,o4)
Y2 <-- (
          1.00000000) V2(c1,c1,m,o1)
Y3 <-- (
           1.00000000) V2(c1,c1,o1,o2)
Y4 <-- (
           1.00000000) V2(c1,c1,o1,o3)
          1.00000000) V2(c1,c1,o1,o3)
Y5 <-- (
Y6 <-- (
          1.00000000) V2(c1,c1,o1,o2)
Y7 <-- (
          1.00000000) V2(c1,c1,i,o3)
          1.00000000) V2(c1,c1,i,o3)
1.00000000) V2(c1,c1,k,o3)
1.00000000) V2(c1,c1,k,o3)
Y8 <-- (
Y9 <-- (
Y10 <-- (
Y11 <-- (
           1.00000000) V2(c1,m,c1,o3)
Y12 <-- (
            1.00000000) V2(c1,o1,c1,o4)
Y13 <-- (
             1.00000000) V2(c1,m,c1,o1)
            1.000000000) V2(c1,o1,c1,o2)
1.00000000) V2(c1,o1,c1,o3)
Y14 <-- (
Y15 <-- (
             1.00000000) V2(c1,o1,c1,o3)
Y16 <-- (
Y17 <-- (
            1.00000000) V2(c1,o1,c1,o2)
Y18 <-- (
            1.00000000) V2(c1,i,c1,o3)
Y19 <-- (
           1.00000000) V2(c1,i,c1,o3)
Y20 <-- (
            1.00000000) V2(c1,k,c1,o3)
            1.00000000) V2(c1,k,c1,o3)
Y21 <-- (
            1.00000000) V2(c1,c1,a,v1)
Y22 <-- (
Y23 <-- (
            1.00000000) V2(c1,c1,a,v1)
Y24 <-- (
            1.00000000) V2(c1,a,c1,v1)
Y25 <-- (
            1.00000000) V2(c1,a,c1,v1)
! No.0
! S2(i,k,m,a) <--
! (0.50000000) D3(i,o3,k,o2,o4,o1) T2(o1,o2,o4,a) h(m,o3)
! Indices of BareAmp are rotated to match with LHS.
Case 0 \ldots X(i,o3,k,a) < ---- (1.00000000) D3(i,o3,k,o2,o4,o1) T2(o1,o2,
o4,a)
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^3)
Case 1 ..... X(i,k,o2,o4,o1,m) < ---- (1.00000000) D3(i,o3,k,o2,o4,o1) h(m
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^6)
Case 2 ..... X(01,02,04,m,03,a) < ---- ( 1.00000000) T2(01,02,04,a) h(m,03)
! Polynomial order is O(o^7v^1)
! Maximum memory usage is O(o^5)
```

```
eclipse sort.dat
  9 11, 12 16:46
                                                                  Page 102/145
! The optimal choice is .....

1: X(i,o3,k,a) <-- ( 1.00000000) D3(i,o3,k,o2,o4,o1) T2(o1,o2,o4,a)

2: S2(i,k,m,a) <-- ( 0.50000000) X(i,o3,k,a) h(m,o3)
! Scaling
              : O(o^6v^1)
! Max size of X : o^3
! * Begin scaling analysis .... *
for a in {vir}:
 Read T2 from GA for a
  Read S2 from GA for a
  Declare X as a o^3 tensor
  X_{(a)}(i,o3,k) += 1.0 sum(o2,o4,o1) D3(i,o3,k,o2,o4,o1) * T2(o1,o2,o4,)
  S2_{(a)}(i,k,m) += 0.5 sum(o3) X_{(a)}(i,o3,k,) * h(m,o3)
 Accumulate S2 (a)(i,k,m) for a
! No.1
! S2(i,k,m,a) <--
! ( 0.50000000) D3(i,m,k,o3,o4,o2) T2(o2,o3,o1,a) h(o4,o1)
! Indices of BareAmp are rotated to match with LHS.
,o3,o1,a)
! Polynomial order is O(o^7v^1)
! Maximum memory usage is O(o^5)
Case 1 ..... X(i,m,k,o3,o2,o1) <---- ( 1.00000000) D3(i,m,k,o3,o4,o2) h(o4)
,01)
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^6)
Case 2 ..... X(o2,o3,o4,a) <---- ( 1.00000000) T2(o2,o3,o1,a) h(o4,o1)
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^3)
Factorize: Conflict between choices of optimal memory usage and polynomial order
! The optimal choice is .....
1: X(i,m,k,o3,o2,o1) < -- ( 1.00000000) D3(i,m,k,o3,o4,o2) h(o4,o1)
2: S2(i,k,m,a) < -- ( 0.50000000) T2(02,03,01,a) \times (i,m,k,03,02,01)
! Scaling
             : O(o^6v^1)
! Max size of X : o^6
! * Begin scaling analysis .... *
Declare X as a o^6 tensor
X_{()}(i,m,k,o3,o2,o1) += 1.0 sum(o4) D3(i,m,k,o3,o4,o2) * h(o4,o1)
for a in {vir}:
 Read S2 from GA for a
  Read T2 from GA for a
  S2_{(a)}(i,k,m) += 0.5 \text{ sum}(02,03,01) T2(02,03,01,) * X_{()}(i,m,k,03,02,01)
  Accumulate S2_(a)(i,k,m) for a
! No.2
! S2(i,k,m,a) <--
! ( 1.00000000) D2(i,o3,k,o2) T2(o3,o2,o1,a) h(m,o1)
! Indices of BareAmp are rotated to match with LHS.
Case 0 ..... X(i,k,o1,a) < ---- ( 1.00000000) D2(i,o3,k,o2) T2(o3,o2,o1,a)
```

```
eclipse sort.dat
 9 11, 12 16:46
                                                                   Page 103/145
! Polynomial order is O(o^5v^1)
! Maximum memory usage is O(o^3)
Case 1 .... X(i,o3,k,o2,m,o1) < ---- ( 1.00000000) D2(i,o3,k,o2) h(m,o1)
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^6)
Case 2 ..... X(03,02,m,a) < ---- ( 1.00000000) T2(03,02,01,a) h(m,o1)
! Polynomial order is O(o^5v^1)
! Maximum memory usage is O(o^3)
! The optimal choice is .....
1: X(i,\tilde{k},o1,a) < -- ( 1.00000000) D2(i,o3,k,o2) T2(o3,o2,o1,a) 2: S2(i,k,m,a) < -- ( 1.00000000) X(i,k,o1,a) h(m,o1)
! Scaling : O(o^5v^1)
! Max size of X : o^3
! * Begin scaling analysis .... *
for a in {vir}:
 Read T2 from GA for a
 Read S2 from GA for a
 Declare X as a o^3 tensor
 X_{(a)}(i,k,o1) += 1.0 sum(o3,o2) D2(i,o3,k,o2) * T2(o3,o2,o1,)
 S2_(a)(i,k,m) += 1.0 sum(o1) X_(a)(i,k,o1,) * h(m,o1)
 Accumulate S2 (a)(i,k,m) for a
! No.3
! S2(i,k,m,a) <--
! ( -0.50000000) D3(i,m,k,o3,o4,o2) T2(o1,o3,o4,a) h(o2,o1)
! Indices of BareAmp are rotated to match with LHS.
! Polynomial order is O(o^7v^1)
! Maximum memory usage is O(o^5)
Case 1 ..... X(i,m,k,o3,o4,o1) <---- ( 1.00000000) D3(i,m,k,o3,o4,o2) h(o2)
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^6)
Case 2 ..... X(03,04,02,a) < ---- (1.00000000) T2(01,03,04,a) h(02,01)
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^3)
Factorize: Conflict between choices of optimal memory usage and polynomial order
! The optimal choice is .....
1: X(i,m,k,o3,o4,o1) <-- ( 1.00000000) D3(i,m,k,o3,o4,o2) h(o2,o1) 
2: S2(i,k,m,a) <-- ( -0.50000000) T2(o1,o3,o4,a) X(i,m,k,o3,o4,o1)
! Scaling
              : O(o^6v^1)
! Max size of X : o^6
! * Begin scaling analysis .... *
Declare X as a o^6 tensor
X_{()}(i,m,k,o3,o4,o1) += 1.0 sum(o2) D3(i,m,k,o3,o4,o2) * h(o2,o1)
for a in {vir}:
 Read S2 from GA for a
 Read T2 from GA for a
 S2_{(a)}(i,k,m) += -0.5 \text{ sum}(01,03,04) T2(01,03,04,) * X_{()}(i,m,k,03,04,01)
 Accumulate S2_(a)(i,k,m) for a
```

```
eclipse sort.dat
  9 11, 12 16:46
                                                                     Page 104/145
! No.4
! S2(i,k,m,a) <--
! ( -0.50000000) D2(i,o3,k,o2) T2(o1,o2,m,a) h(o3,o1)
! Indices of BareAmp are rotated to match with LHS.
Case 0 ..... X(i,o3,k,o1,m,a) <---- ( 1.00000000) D2(i,o3,k,o2) T2(o1,o2,m
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^5)
Case 1 .... X(i,k,o2,o1) < ---- (1.00000000) D2(i,o3,k,o2) h(o3,o1)
! Polynomial order is O(o^5v^1)
! Maximum memory usage is O(o^4)
Case 2 ..... X(o2,m,o3,a) < ---- ( 1.00000000) T2(o1,o2,m,a) h(o3,o1)
! Polynomial order is O(o^5v^1)
! Maximum memory usage is O(o^3)
Factorize: Conflict between choices of optimal memory usage and polynomial order
! The optimal choice is .....
1: X(i,k,02,01) <-- ( 1.00000000) D2(i,03,k,02) h(03,01) 
2: S2(i,k,m,a) <-- ( -0.50000000) T2(o1,02,m,a) X(i,k,02,01)
! Scaling : O(o^5v^1)
! Max size of X : o^4
! * Begin scaling analysis .... *
Declare X as a o^4 tensor
X_{()}(i,k,o2,o1) += 1.0 sum(o3) D2(i,o3,k,o2) * h(o3,o1)
for a in {vir}:
  Read S2 from GA for a
  Read T2 from GA for a
  S2_{(a)(i,k,m)} += -0.5 sum(o1,o2) T2(o1,o2,m,) * X_{(i,k,o2,o1)}
  Accumulate S2_(a)(i,k,m) for a
1 No. 5
! S2(i,k,m,a) <--
! ( -0.50000000) D3(i,m,k,o3,o4,o2) T2(o2,o1,o4,a) h(o3,o1)
! Indices of BareAmp are rotated to match with LHS.
Case 0 ..... X(i,m,k,o3,o1,a) <---- ( 1.00000000) D3(i,m,k,o3,o4,o2) T2(o2
.o1.o4.a)
! Polynomial order is O(o^7v^1)
! Maximum memory usage is O(o^5)
Case 1 .... X(i,m,k,04,02,01) < ---- ( 1.00000000) D3(i,m,k,03,04,02) h(03)
,01)
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^6)
Case 2 ..... X(02,04,03,a) < ---- ( 1.00000000) T2(02,01,04,a) h(03,01)
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^3)
Factorize: Conflict between choices of optimal memory usage and polynomial order
! The optimal choice is .....
1: X(i,m,k,o4,o2,o1) <-- ( 1.00000000) D3(i,m,k,o3,o4,o2) h(o3,o1) 2: S2(i,k,m,a) <-- ( -0.50000000) T2(o2,o1,o4,a) X(i,m,k,o4,o2,o1)
! Scaling
              : O(o^6v^1)
! Max size of X : o^6
```

```
eclipse sort.dat
 9 11, 12 16:46
                                                                   Page 105/145
! * Begin scaling analysis .... *
Declare X as a o^6 tensor
X()(i,m,k,04,02,01) += 1.0 sum(03) D3(i,m,k,03,04,02) * h(03,01)
for a in {vir}:
 Read S2 from GA for a
 Read T2 from GA for a
 S2_{(a)}(i,k,m) += -0.5 sum(o2,o1,o4) T2(o2,o1,o4,) * X_{(i)}(i,m,k,o4,o2,o1)
 Accumulate S2 (a)(i,k,m) for a
! S2(i,k,m,a) <--
! ( -0.50000000) D2(i,o3,k,o2) T2(o3,o1,m,a) h(o2,o1)
! Indices of BareAmp are rotated to match with LHS.
Case 0 ..... X(i,k,o2,o1,m,a) < ---- (1.00000000) D2(i,o3,k,o2) T2(o3,o1,m)
,a)
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^5)
Case 1 ..... X(i,03,k,01) < ---- ( 1.00000000) D2(i,03,k,02) h(02,01)
! Polynomial order is O(o^5v^1)
! Maximum memory usage is O(o^4)
Case 2 ..... X(o3,m,o2,a) <---- ( 1.00000000) T2(o3,o1,m,a) h(o2,o1)
! Polynomial order is O(o^5v^1)
! Maximum memory usage is O(o^3)
Factorize: Conflict between choices of optimal memory usage and polynomial order
! The optimal choice is .....
1: X(i,03,k,01) < -- ( 1.00000000) D2(i,03,k,02) h(02,01) 2: S2(i,k,m,a) < -- ( -0.50000000) T2(03,01,m,a) X(i,03,k,01)
! Scaling
              : O(o^5v^1)
! Max size of X : o^4
! * Begin scaling analysis .... *
Declare X as a o^4 tensor
X_{()}(i,o3,k,o1) += 1.0 sum(o2) D2(i,o3,k,o2) * h(o2,o1)
for a in {vir}:
 Read S2 from GA for a
 Read T2 from GA for a
 S2_{(a)}(i,k,m) += -0.5 \text{ sum}(03,01) T2(03,01,m,) * X_{((i,03,k,01))}
 Accumulate S2_(a)(i,k,m) for a
! No.7
! S2(i,k,m,a) <--
! ( -0.50000000) D3(k,o4,o1,m,o2,o3) T2(o3,o4,o2,a) h(i,o1)
! Indices of BareAmp are rotated to match with LHS.
Case 0 ..... X(k,o1,m,a) <---- ( 1.00000000) D3(k,o4,o1,m,o2,o3) T2(o3,o4,
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^3)
Case 1 ..... X(k,04,m,02,03,i) < ---- (1.00000000) D3(k,04,01,m,02,03) h(i)
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^6)
Case 2 ..... X(03,04,02,i,01,a) < ---- ( 1.00000000) T2(03,04,02,a) h(i,o1)
```

```
eclipse sort.dat
  9 11, 12 16:46
                                                               Page 106/145
! Polynomial order is O(o^7v^1)
! Maximum memory usage is O(o^5)
! The optimal choice is .....
1: X(k,01,m,a) \leftarrow (1.00000000) D3(k,04,01,m,02,03) T2(03,04,02,a)
2: S2(i,k,m,a) < -- (-0.50000000) X(k,o1,m,a) h(i,o1)
! Scaling
            : O(o^6v^1)
! Max size of X : o^3
! * Begin scaling analysis .... *
for a in {vir}:
  Read T2 from GA for a
  Read S2 from GA for a
  Declare X as a o^3 tensor
  X (a)(k,o1,m) += 1.0 sum(o4,o2,o3) D3(k,o4,o1,m,o2,o3) * T2(o3,o4,o2,)
  S2_{(a)}(i,k,m) += -0.5 sum(o1) X_{(a)}(k,o1,m,) * h(i,o1)
  Accumulate S2 (a)(i,k,m) for a
! No.8
! S2(i,k,m,a) <--
! ( -0.50000000) D2(k,o3,o1,o2) T2(o2,o3,m,a) h(i,o1)
! Indices of BareAmp are rotated to match with LHS.
Case 0 ..... X(k,o1,m,a) < ---- (1.00000000) D2(k,o3,o1,o2) T2(o2,o3,m,a)
! Polynomial order is O(o^5v^1)
! Maximum memory usage is O(o^3)
Case 1 .... X(k,03,02,i) <---- ( 1.00000000) D2(k,03,01,02) h(i,01)
! Polynomial order is O(o^5v^1)
! Maximum memory usage is O(o^4)
Case 2 ..... X(o2,o3,m,i,o1,a) < ---- ( 1.00000000) T2(o2,o3,m,a) h(i,o1)
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^5)
! The optimal choice is .....
1: X(k,o1,m,a) < -- ( 1.00000000) D2(k,o3,o1,o2) T2(o2,o3,m,a)
2: S2(i,k,m,a) < -- ( -0.50000000) X(k,o1,m,a) h(i,o1)
! Scaling : O(o^5v^1)
! Max size of X : o^3
! * Begin scaling analysis .... *
for a in {vir}:
  Read T2 from GA for a
  Read S2 from GA for a
  Declare X as a o^3 tensor
  X_{(a)}(k,o1,m) += 1.0 \text{ sum}(o3,o2) D2(k,o3,o1,o2) * T2(o2,o3,m,)
  S2_{(a)}(i,k,m) += -0.5 sum(o1) X_{(a)}(k,o1,m,) * h(i,o1)
  Accumulate S2_(a)(i,k,m) for a
! No.9
! S2(i,k,m,a) <--
[ (-0.50000000) D3(i,m,o3,o1,o4,o2) T2(o2,o1,o4,a) h(k,o3) ]
! Indices of BareAmp are rotated to match with LHS.
```

```
eclipse sort.dat
 9 11, 12 16:46
                                                                     Page 107/145
o4,a)
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^3)
Case 1 ..... X(i,m,o1,o4,o2,k) < ---- (1.00000000) D3(i,m,o3,o1,o4,o2) h(k
,03)
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^6)
Case 2 ..... X(02,01,04,k,03,a) < ---- ( 1.00000000) T2(02,01,04,a) h(k,03)
! Polynomial order is O(o^7v^1)
! Maximum memory usage is O(o^5)
! The optimal choice is .....
1: X(i,m,o3,a) <-- ( 1.00000000) D3(i,m,o3,o1,o4,o2) T2(o2,o1,o4,a)

2: S2(i,k,m,a) <-- ( -0.50000000) X(i,m,o3,a) h(k,o3)
              : O(o^6v^1)
! Scaling
! Max size of X : o^3
! * Begin scaling analysis .... *
for a in {vir}:
   Read T2 from GA for a
 Read S2 from GA for a
 Declare X as a o^3 tensor
 X_{(a)}(i,m,o3) += 1.0 sum(o1,o4,o2) D3(i,m,o3,o1,o4,o2) * T2(o2,o1,o4,)
 S2 (a)(i,k,m) += -0.5 sum(o3) X (a)(i,m,o3,) * h(k,o3)
 Accumulate S2 (a)(i,k,m) for a
! No.10
! S2(i,k,m,a) <--
! (-0.50000000) D2(i,02,03,01) T2(02,01,m,a) h(k,03)
! Indices of BareAmp are rotated to match with LHS.
Case 0 ..... X(i,o3,m,a) < ---- (1.00000000) D2(i,o2,o3,o1) T2(o2,o1,m,a)
! Polynomial order is O(o^5v^1)
! Maximum memory usage is O(o^3)
Case 1 .... X(i,02,01,k) < ---- (1.00000000) D2(i,02,03,01) h(k,03)
! Polynomial order is O(o^5v^1)
! Maximum memory usage is O(o^4)
Case 2 .... X(02.01,m,k,03.a) < ---- ( 1.00000000) T2(02.01,m,a) h(k,03)
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^5)
! The optimal choice is .....
1: X(i,03,m,a) < -- ( 1.00000000) D2(i,02,03,01) T2(02,01,m,a) 2: S2(i,k,m,a) < -- ( -0.50000000) X(i,03,m,a) h(k,03)
! Scaling
              : O(o^5v^1)
! Max size of X : o^3
! * Begin scaling analysis .... *
for a in {vir}:
 Read T2 from GA for a
 Read S2 from GA for a
 Declare X as a o^3 tensor
 X_{(a)}(i,o3,m) += 1.0 sum(o2,o1) D2(i,o2,o3,o1) * T2(o2,o1,m,)
 S2_{(a)}(i,k,m) += -0.5 sum(o3) X_{(a)}(i,o3,m,) * h(k,o3)
 Accumulate S2_(a)(i,k,m) for a
```

```
eclipse sort.dat
  9 11, 12 16:46
                                                                     Page 108/145
! S2(i,k,m,a) <--
! ( 1.00000000) D3(i,m,k,o2,o1,o3) T2(o3,o2,o1,v1) h(a,v1)
Case 0 ..... X(i,m,k,v1) < ---- (1.00000000) D3(i,m,k,o2,o1,o3) T2(o3,o2,o
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^3)
Case 1 ..... X(i,m,k,o2,o1,o3,a,v1) < ---- (1.00000000) D3(i,m,k,o2,o1,o3)
! Polynomial order is O(o^6v^2)
! Maximum memory usage is O(o^6)
Case 2 ..... X(03,02,01,a) < ---- ( 1.00000000) T2(03,02,01,v1) h(a,v1)
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^3)
! The optimal choice is .....
1: X(i,m,k,v1) < -- ( 1.00000000) D3(i,m,k,o2,o1,o3) T2(o3,o2,o1,v1) 2: S2(i,k,m,a) < -- ( 1.00000000) X(i,m,k,v1) h(a,v1)
! Scaling
             : O(o^6v^1)
! Max size of X : o^3
! * Begin scaling analysis .... *
for v1 in {vir}:
 Read T2 from GA for v1
  Declare X as a o^3 tensor
  X(v1)(i,m,k) += 1.0 sum(o2,o1,o3) D3(i,m,k,o2,o1,o3) * T2(o3,o2,o1,)
  for a in {vir}:
   Read S2 from GA for a
    S2 (a)(i,k,m) += 1.0 sum() X (v1)(i,m,k,) * h(a,v1)
   Accumulate S2 (a)(i,k,m) for a
! S2(i,k,m,a) <--
! ( 1.00000000) D2(i,o1,k,o2) T2(o1,o2,m,v1) h(a,v1)
Case 0 ..... X(i,k,m,v1) < ---- ( 1.00000000) D2(i,o1,k,o2) T2(o1,o2,m,v1)
! Polynomial order is O(o^5v^1)
! Maximum memory usage is O(o^3)
Case 1 ..... X(i,01,k,02,a,v1) < ---- ( 1.00000000) D2(i,01,k,02) h(a,v1)
! Polynomial order is O(o^5v^2)
! Maximum memory usage is O(o^4)
Case 2 ..... X(01,02,m,a) < ---- (1.00000000) T2(01,02,m,v1) h(a,v1)
! Polynomial order is O(o^5v^1)
! Maximum memory usage is O(o^3)
! The optimal choice is .....
1: X(i,k,m,v1) <-- ( 1.00000000) D2(i,o1,k,o2) T2(o1,o2,m,v1)
2: S2(i,k,m,a) <-- ( 1.00000000) X(i,k,m,v1) h(a,v1)
! Scaling : 0(o^5v^1)
! Max size of X : o^3
! * Begin scaling analysis .... *
for v1 in {vir}:
 Read T2 from GA for v1
  Declare X as a o^3 tensor
  X_{(v1)}(i,k,m) += 1.0 \text{ sum}(01,02) D2(i,01,k,02) * T2(01,02,m,)
```

```
eclipse sort.dat
 9 11, 12 16:46
                                                                   Page 109/145
  for a in {vir}:
    Read S2 from GA for a
    S2 (a)(i,k,m) += 1.0 sum() X (v1)(i,k,m,) * h(a,v1)
    Accumulate S2 (a)(i,k,m) for a
! No.13
! S2(i,k,m,a) <--
! (1.00000000) D3(i,o3,k,o2,o4,o1) T2(o1,o2,o4,a) Y0(m,o3)
! Indices of BareAmp are rotated to match with LHS.
Case 0 ..... X(i,o3,k,a) <---- ( 1.00000000) D3(i,o3,k,o2,o4,o1) T2(o1,o2,
o4,a)
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^3)
Case 1 ..... X(i,k,o2,o4,o1,m) < ---- ( 1.00000000) D3(i,o3,k,o2,o4,o1) Y0(
m, o3)
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^6)
Case 2 ..... X(01,02,04,m,03,a) < ---- (1.00000000) T2(01,02,04,a) Y0(m,03)
! Polynomial order is O(o^7v^1)
! Maximum memory usage is O(o^5)
! The optimal choice is .....
1: X(i,o3,k,a) < -- ( 1.00000000) D3(i,o3,k,o2,o4,o1) T2(o1,o2,o4,a) 2: S2(i,k,m,a) < -- ( 1.00000000) X(i,o3,k,a) Y0(m,o3)
              : O(o^6v^1)
! Max size of X : o^3
! * Begin scaling analysis .... *
Declare Y0 as a tensor
for c1 in {core}:
 Read V2 from GA for c1
for a in {vir}:
 Read T2 from GA for a
 Read S2 from GA for a
 Declare X as a o^3 tensor
 X_{(a)}(i,03,k) += 1.0 sum(02,04,01) D3(i,03,k,02,04,01) * T2(01,02,04,)
 S2_{(a)}(i,k,m) += 1.0 sum(o3) X_{(a)}(i,o3,k,) * Y0(m,o3)
 Accumulate S2_(a)(i,k,m) for a
! No.14
! S2(i,k,m,a) <--
! ( 1.00000000) D3(i,m,k,o3,o4,o2) T2(o2,o3,o1,a) Y1(o1,o4)
! Indices of BareAmp are rotated to match with LHS.
Case 0 ..... X(i,m,k,o4,o1,a) < ---- (1.00000000) D3(i,m,k,o3,o4,o2) T2(o2)
.o3.o1.a)
! Polynomial order is O(o^7v^1)
! Maximum memory usage is O(o^5)
Case 1 .... X(i,m,k,o3,o2,o1) <---- ( 1.00000000) D3(i,m,k,o3,o4,o2) Y1(o
1,04)
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^6)
Case 2 .... X(02,03,04,a) < ---- ( 1.00000000) T2(02,03,01,a) Y1(01,04)
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^3)
```

```
eclipse sort.dat
  9 11, 12 16:46
                                                                       Page 110/145
Factorize: Conflict between choices of optimal memory usage and polynomial order
! The optimal choice is .....
1: X(i,m,k,o3,o2,o1) <-- ( 1.00000000) D3(i,m,k,o3,o4,o2) Y1(o1,o4) 
2: S2(i,k,m,a) <-- ( 1.00000000) T2(o2,o3,o1,a) X(i,m,k,o3,o2,o1)
               : O(o^6v^1)
! Max size of X : o^6
! * Begin scaling analysis .... *
Declare Y1 as a tensor
for c1 in {core}:
 Read V2 from GA for c1
Declare X as a o^6 tensor
X()(i,m,k,o3,o2,o1) += 1.0 sum(o4) D3(i,m,k,o3,o4,o2) * Y1(o1,o4)
for a in {vir}:
 Read S2 from GA for a
  Read T2 from GA for a
  S2_{(a)}(i,k,m) += 1.0 sum(02,03,01) T2(02,03,01,) * X_{()}(i,m,k,03,02,01)
  Accumulate S2 (a)(i,k,m) for a
! No.15
! S2(i,k,m,a) <--
! ( 2.00000000) D2(i,o3,k,o2) T2(o3,o2,o1,a) Y2(m,o1)
! Indices of BareAmp are rotated to match with LHS.
Case 0 ..... X(i,k,o1,a) < ---- (1.00000000) D2(i,o3,k,o2) T2(o3,o2,o1,a)
! Polynomial order is O(o^5v^1)
! Maximum memory usage is O(o^3)
Case 1 .... X(i,o3,k,o2,m,o1) < ---- (1.00000000) D2(i,o3,k,o2) Y2(m,o1)
! Polynomial order is O(o^6v^1)
 ! Maximum memory usage is O(o^6)
Case 2 ..... X(03,02,m,a) < ---- (1.00000000) T2(03,02,01,a) Y2(m,o1)
! Polynomial order is O(o^5v^1)
! Maximum memory usage is O(o^3)
! The optimal choice is .....
1: X(i,k,o1,a) <-- ( 1.00000000) D2(i,o3,k,o2) T2(o3,o2,o1,a)
2: S2(i,k,m,a) <-- ( 2.00000000) X(i,k,o1,a) Y2(m,o1)
              : O(o^5v^1)
! Max size of X : o^3
! * Begin scaling analysis .... *
Declare Y2 as a tensor
for c1 in {core}:
 Read V2 from GA for cl
for a in {vir}:
  Read T2 from GA for a
  Read S2 from GA for a
  Declare X as a o^3 tensor
  X_{(a)}(i,k,o1) += 1.0 \text{ sum}(o3,o2) D2(i,o3,k,o2) * T2(o3,o2,o1,)
  S2_{(a)}(i,k,m) += 2 sum(o1) X_{(a)}(i,k,o1,) * Y2(m,o1)
  Accumulate S2_(a)(i,k,m) for a
```

```
9 11, 12 16:46
                               eclipse sort.dat
                                                                   Page 111/145
! No.16
! S2(i,k,m,a) <--
! (-1.00000000) D3(i,m,k,o3,o4,o2) T2(o1,o3,o4,a) Y3(o1,o2)
! Indices of BareAmp are rotated to match with LHS.
! Polynomial order is O(o^7v^1)
! Maximum memory usage is O(o^5)
Case 1 ..... X(i,m,k,o3,o4,o1) < ---- (1.00000000) D3(i,m,k,o3,o4,o2) Y3(o
1,02)
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^6)
Case 2 ..... X(o3,o4,o2,a) <---- ( 1.00000000) T2(o1,o3,o4,a) Y3(o1,o2)
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^3)
Factorize: Conflict between choices of optimal memory usage and polynomial order
! The optimal choice is .....
1: X(i,m,k,o3,o4,o1) <-- ( 1.00000000) D3(i,m,k,o3,o4,o2) Y3(o1,o2)
2: S2(i,k,m,a) <-- ( -1.00000000) T2(o1,o3,o4,a) X(i,m,k,o3,o4,o1)
              : O(o^6v^1)
! Max size of X : o^6
! * Begin scaling analysis .... *
Declare Y3 as a tensor
for c1 in {core}:
 Read V2 from GA for c1
Declare X as a o^6 tensor
X()(i,m,k,o3,o4,o1) += 1.0 sum(o2) D3(i,m,k,o3,o4,o2) * Y3(o1,o2)
for a in {vir}:
  Read S2 from GA for a
  Read T2 from GA for a
 S2 (a)(i,k,m) += -1 sum(o1,o3,o4) T2(o1,o3,o4,) * X_()(i,m,k,o3,o4,o1)
 Accumulate S2_(a)(i,k,m) for a
! No.17
! S2(i,k,m,a) < --
! (-1.00000000) D2(i,o3,k,o2) T2(o1,o2,m,a) Y4(o1,o3)
! Indices of BareAmp are rotated to match with LHS.
Case 0 ..... X(i,o3,k,o1,m,a) < ---- ( 1.00000000) D2(i,o3,k,o2) T2(o1,o2,m)
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^5)
Case 1 ..... X(i,k,o2,o1) < ---- (1.00000000) D2(i,o3,k,o2) Y4(o1,o3)
! Polynomial order is O(o^5v^1)
! Maximum memory usage is O(o^4)
Case 2 ..... X(02,m,03,a) <---- ( 1.00000000) T2(01,02,m,a) Y4(01,03)
! Polynomial order is O(o^5v^1)
! Maximum memory usage is O(o^3)
Factorize: Conflict between choices of optimal memory usage and polynomial order
! The optimal choice is .....
1: X(i,k,o2,o1) <-- ( 1.0000000) D2(i,o3,k,o2) Y4(o1,o3)
2: S2(i,k,m,a) <-- ( -1.0000000) T2(o1,o2,m,a) X(i,k,o2,o1)
! Scaling
               : O(o^5v^1)
```

```
eclipse sort.dat
  9 11, 12 16:46
                                                                 Page 112/145
! Max size of X : o^4
! * Begin scaling analysis .... *
Declare Y4 as a tensor
for cl in {core}:
 Read V2 from GA for c1
Declare X as a o^4 tensor
X()(i,k,o2,o1) += 1.0 sum(o3) D2(i,o3,k,o2) * Y4(o1,o3)
for a in {vir}:
  Read S2 from GA for a
  Read T2 from GA for a
  S2_{(a)}(i,k,m) += -1 sum(o1,o2) T2(o1,o2,m,) * X_{(i,k,o2,o1)}
  Accumulate S2 (a)(i,k,m) for a
! S2(i,k,m,a) <--
! (-1.00000000) D3(i,m,k,o3,o4,o2) T2(o2,o1,o4,a) Y5(o1,o3)
! Indices of BareAmp are rotated to match with LHS.
,o1,o4,a)
! Polynomial order is O(o^7v^1)
! Maximum memory usage is O(o^5)
Case 1 .... X(i,m,k,o4,o2,o1) < ---- ( 1.00000000) D3(i,m,k,o3,o4,o2) Y5(o
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^6)
Case 2 ..... X(02,04,03,a) < ---- ( 1.00000000) T2(02,01,04,a) Y5(01,03)
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^3)
Factorize: Conflict between choices of optimal memory usage and polynomial order
! The optimal choice is .....
1: X(i,m,k,o4,o2,o1) <-- ( 1.00000000) D3(i,m,k,o3,o4,o2) Y5(o1,o3) 
2: S2(i,k,m,a) <-- ( -1.00000000) T2(o2,o1,o4,a) X(i,m,k,o4,o2,o1)
! Scaling
             : O(o^6v^1)
! Max size of X : o^6
! * Begin scaling analysis .... *
Declare Y5 as a tensor
for c1 in {core}:
 Read V2 from GA for c1
Declare X as a o^6 tensor
X_{()}(i,m,k,o4,o2,o1) += 1.0 sum(o3) D3(i,m,k,o3,o4,o2) * Y5(o1,o3)
for a in {vir}:
 Read S2 from GA for a
  Read T2 from GA for a
  S2_{(a)}(i,k,m) += -1 sum(o2,o1,o4) T2(o2,o1,o4,) * X_{((i,m,k,o4,o2,o1))}
 Accumulate S2_(a)(i,k,m) for a
! No.19
! S2(i,k,m,a) <--
```

```
eclipse sort.dat
 9 11, 12 16:46
                                                                  Page 113/145
! ( -1.00000000) D2(i,o3,k,o2) T2(o3,o1,m,a) Y6(o1,o2)
! Indices of BareAmp are rotated to match with LHS.
Case 0 ..... X(i,k,o2,o1,m,a) < ---- (1.00000000) D2(i,o3,k,o2) T2(o3,o1,m)
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^5)
Case 1 ..... X(i,03,k,01) < ---- (1.00000000) D2(i,03,k,02) Y6(01,02)
! Polynomial order is O(o^5v^1)
! Maximum memory usage is O(o^4)
Case 2 ..... X(o3,m,o2,a) <---- ( 1.00000000) T2(o3,o1,m,a) Y6(o1,o2)
! Polynomial order is O(o^5v^1)
! Maximum memory usage is O(o^3)
Factorize: Conflict between choices of optimal memory usage and polynomial order
! The optimal choice is .....
1: X(i,03,k,01) < -- ( 1.00000000) D2(i,03,k,02) Y6(01,02) 2: S2(i,k,m,a) < -- ( -1.00000000) T2(03,01,m,a) X(i,03,k,01)
             : O(o^5v^1)
! Scaling
! Max size of X : o^4
! * Begin scaling analysis .... *
Declare Y6 as a tensor
for c1 in {core}:
 Read V2 from GA for c1
Declare X as a o^4 tensor
X_{()}(i,o3,k,o1) += 1.0 sum(o2) D2(i,o3,k,o2) * Y6(o1,o2)
for a in {vir}:
 Read S2 from GA for a
 Read T2 from GA for a
 S2 (a)(i,k,m) += -1 sum(03,01) T2(03,01,m,) * X ()(i,03,k,01)
 Accumulate S2 (a)(i,k,m) for a
! No. 20
! S2(i,k,m,a) <--
! (-1.00000000) D3(k,02,03,m,04,01) T2(01,02,04,a) Y7(i,03)
! Indices of BareAmp are rotated to match with LHS.
o4,a)
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^3)
Case 1 ..... X(k,o2,m,o4,o1,i) <---- ( 1.00000000) D3(k,o2,o3,m,o4,o1) Y7(
i,03)
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^6)
Case 2 ..... X(01,02,04,i,03,a) < ---- (1.00000000) T2(01,02,04,a) Y7(i,03)
! Polynomial order is O(o^7v^1)
! Maximum memory usage is O(o^5)
! The optimal choice is .....
1: X(k,03,m,a) < -- ( 1.00000000) D3(k,02,03,m,04,01) T2(01,02,04,a) 2: S2(i,k,m,a) < -- ( -1.00000000) X(k,03,m,a) Y7(i,03)
! Scaling
              : O(o^6v^1)
! Max size of X : o^3
! * Begin scaling analysis .... *
Declare Y7 as a tensor
```

```
eclipse sort.dat
  9 11, 12 16:46
                                                                     Page 114/145
for c1 in {core}:
  Read V2 from GA for c1
for a in {vir}:
  Read T2 from GA for a
  Read S2 from GA for a
  Declare X as a o^3 tensor
  X_{(a)}(k,o3,m) += 1.0 sum(o2,o4,o1) D3(k,o2,o3,m,o4,o1) * T2(o1,o2,o4,)
  S2 (a)(i,k,m) += -1 sum(o3) X (a)(k,o3,m,) * Y7(i,o3)
  Accumulate S2_(a)(i,k,m) for a
I No 21
! S2(i,k,m,a) <--
! (-1.00000000) D2(k,o2,o3,o1) T2(o1,o2,m,a) Y8(i,o3)
! Indices of BareAmp are rotated to match with LHS.
Case 0 ..... X(k,o3,m,a) < ---- ( 1.00000000) D2(k,o2,o3,o1) T2(o1,o2,m,a)
! Polynomial order is O(o^5v^1)
! Maximum memory usage is O(o^3)
Case 1 ..... X(k,02,01,i) <---- ( 1.00000000) D2(k,02,03,01) Y8(i,03)
! Polynomial order is O(o^5v^1)
! Maximum memory usage is O(o^4)
Case 2 ..... X(01,02,m,i,03,a) < ---- (1.00000000) T2(01,02,m,a) Y8(i,03)
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^5)
! The optimal choice is .....
1: X(k,03,m,a) < -- ( 1.00000000) D2(k,02,03,01) T2(01,02,m,a)
2: S2(i,k,m,a) < -- ( -1.00000000) X(k,03,m,a) Y8(i,03)
! Scaling
             : O(o^5v^1)
! Max size of X : o^3
! * Begin scaling analysis .... *
Declare Y8 as a tensor
for c1 in {core}:
  Read V2 from GA for c1
for a in {vir}:
  Read T2 from GA for a
  Read S2 from GA for a
  Declare X as a o^3 tensor
  X_{(a)}(k,o3,m) += 1.0 \text{ sum}(o2,o1) D2(k,o2,o3,o1) * T2(o1,o2,m,)
  S2_{(a)}(i,k,m) += -1 sum(o3) X_{(a)}(k,o3,m,) * Y8(i,o3)
  Accumulate S2_(a)(i,k,m) for a
! No.22
! S2(i,k,m,a) <--
[ (-1.00000000) D3(i,m,o3,o1,o4,o2) T2(o2,o1,o4,a) Y9(k,o3) ]
! Indices of BareAmp are rotated to match with LHS.
Case 0 ..... X(i,m,o3,a) <---- ( 1.00000000) D3(i,m,o3,o1,o4,o2) T2(o2,o1,
o4,a)
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^3)
Case 1 ..... X(\bar{1}, m, o\bar{1}, o4, o2, k) < ---- ( 1.00000000) D3(i, m, o3, o1, o4, o2) Y9(
! Polynomial order is O(o^6v^1)
```

```
eclipse sort.dat
 9 11, 12 16:46
                                                                      Page 115/145
! Maximum memory usage is O(o^6)
Case 2 ..... X(02,01,04,k,03,a) < ---- ( 1.00000000) T2(02,01,04,a) Y9(k,03)
! Polynomial order is O(o^7v^1)
! Maximum memory usage is O(o^5)
! The optimal choice is .....
1: X(i,m,o3,a) <-- ( 1.00000000) D3(i,m,o3,o1,o4,o2) T2(o2,o1,o4,a) 2: S2(i,k,m,a) <-- ( -1.00000000) X(i,m,o3,a) Y9(k,o3)
! Scaling : O(o^6v^1)
! Max size of X : o^3
! * Begin scaling analysis .... *
Declare Y9 as a tensor
for c1 in {core}:
 Read V2 from GA for c1
for a in {vir}:
 Read T2 from GA for a
 Read S2 from GA for a
 Declare X as a o^3 tensor
 X(a)(i,m,o3) += 1.0 sum(o1,o4,o2) D3(i,m,o3,o1,o4,o2) * T2(o2,o1,o4,)
 S2_{(a)}(i,k,m) += -1 sum(o3) X_{(a)}(i,m,o3,) * Y9(k,o3)
 Accumulate S2 (a)(i,k,m) for a
! No.23
! S2(i,k,m,a) <--
! (-1.00000000) D2(i,o2,o3,o1) T2(o2,o1,m,a) Y10(k,o3)
! Indices of BareAmp are rotated to match with LHS.
Case 0 \dots X(i, o3, m, a) < ---- (1.00000000) D2(i, o2, o3, o1) T2(o2, o1, m, a)
! Polynomial order is O(o^5v^1)
! Maximum memory usage is O(o^3)
Case 1 ..... X(i,02,01,k) < ---- (1.00000000) D2(i,02,03,01) Y10(k,03)
! Polynomial order is O(o^5v^1)
! Maximum memory usage is O(o^4)
Case 2 ..... X(o2,o1,m,k,o3,a) <---- ( 1.00000000) T2(o2,o1,m,a) Y10(k,o3)
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^5)
! The optimal choice is .....
1: X(i,03,m,a) < -- ( 1.00000000) D2(i,02,03,01) T2(02,01,m,a)
2: S2(i,k,m,a) < -- ( -1.00000000) X(i,03,m,a) Y10(k,03)
! Scaling
              : O(o^5v^1)
! Max size of X : o^3
! * Begin scaling analysis .... *
Declare Y10 as a tensor
for c1 in {core}:
 Read V2 from GA for cl
for a in {vir}:
 Read T2 from GA for a
 Read S2 from GA for a
 Declare X as a o^3 tensor
 X_{(a)}(i,o3,m) += 1.0 \text{ sum}(o2,o1) D2(i,o2,o3,o1) * T2(o2,o1,m,)
 S2_{(a)}(i,k,m) += -1 sum(o3) X_{(a)}(i,o3,m,) * Y10(k,o3)
```

```
eclipse sort.dat
  9 11, 12 16:46
                                                                 Page 116/145
  Accumulate S2 (a)(i,k,m) for a
! No.24
! S2(i,k,m,a) <--
! ( -0.50000000) D3(i,o3,k,o2,o4,o1) T2(o1,o2,o4,a) Y11(m,o3)
! Indices of BareAmp are rotated to match with LHS.
Case 0 \dots X(i, 03, k, a) < ---- (1.00000000) D3(i, 03, k, 02, 04, 01) T2(01, 02,
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^3)
Case 1 ..... X(i,k,o2,o4,o1,m) <---- ( 1.00000000) D3(i,o3,k,o2,o4,o1) Y11
(m, o3)
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^6)
Case 2 ..... X(01,02,04,m,03,a) < ---- (1.00000000) T2(01,02,04,a) Y11(m,0)
! Polynomial order is O(o^7v^1)
! Maximum memory usage is O(o^5)
! The optimal choice is .....
1: X(i,03,k,a) < -- ( 1.00000000) D3(i,03,k,02,04,01) T2(01,02,04,a) 2: S2(i,k,m,a) < -- ( -0.50000000) X(i,03,k,a) Y11(m,03)
! Scaling
             : O(o^6v^1)
! Max size of X : o^3
! * Begin scaling analysis .... *
Declare Y11 as a tensor
for c1 in {core}:
 Read V2 from GA for c1
for a in {vir}:
  Read T2 from GA for a
  Read S2 from GA for a
  Declare X as a o^3 tensor
  X_{(a)}(i,o3,k) += 1.0 sum(o2,o4,o1) D3(i,o3,k,o2,o4,o1) * T2(o1,o2,o4,)
  S2 (a)(i,k,m) += -0.5 sum(o3) X_(a)(i,o3,k,) * Y11(m,o3)
  Accumulate S2_(a)(i,k,m) for a
! No.25
! S2(i,k,m,a) <--
! (-0.50000000) D3(i,m,k,o3,o4,o2) T2(o2,o3,o1,a) Y12(o1,o4)
! Indices of BareAmp are rotated to match with LHS.
.03.01.a)
! Polynomial order is O(o^7v^1)
! Maximum memory usage is O(o^5)
Case 1 ..... X(i,m,k,o3,o2,o1) < ---- (1.00000000) D3(i,m,k,o3,o4,o2) Y12(
01.04
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^6)
Case 2 ..... X(02,03,04,a) < ---- ( 1.00000000) T2(02,03,01,a) Y12(01,04)
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^3)
Factorize: Conflict between choices of optimal memory usage and polynomial order
! The optimal choice is .....
```

```
eclipse sort.dat
 9 11, 12 16:46
                                                                   Page 117/145
1: X(i,m,k,o3,o2,o1) < -- (1.00000000) D3(i,m,k,o3,o4,o2) Y12(o1,o4)
2: S2(i,k,m,a) < -- ( -0.50000000) T2(o2,o3,o1,a) X(i,m,k,o3,o2,o1)
              : O(o^6v^1)
! Max size of X : o^6
! * Begin scaling analysis .... *
Declare Y12 as a tensor
for c1 in {core}:
 Read V2 from GA for c1
Declare X as a o^6 tensor
X()(i,m,k,o3,o2,o1) += 1.0 sum(o4) D3(i,m,k,o3,o4,o2) * Y12(o1,o4)
for a in {vir}:
 Read S2 from GA for a
 Read T2 from GA for a
 S2(a)(i,k,m) += -0.5 sum(02,03,01) T2(02,03,01,) * X()(i,m,k,03,02,01)
 Accumulate S2 (a)(i,k,m) for a
! No.26
! S2(i,k,m,a) <--
! (-1.00000000) D2(i,o3,k,o2) T2(o3,o2,o1,a) Y13(m,o1)
! Indices of BareAmp are rotated to match with LHS.
Case 0 ..... X(i,k,o1,a) < ---- (1.00000000) D2(i,o3,k,o2) T2(o3,o2,o1,a)
! Polynomial order is O(o^5v^1)
! Maximum memory usage is O(o^3)
Case 1 ..... X(i,03,k,02,m,01) < ---- (1.00000000) D2(i,03,k,02) Y13(m,01)
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^6)
Case 2 ..... X(o3,o2,m,a) <---- ( 1.00000000) T2(o3,o2,o1,a) Y13(m,o1)
! Polynomial order is O(o^5v^1)
! Maximum memory usage is O(o^3)
! The optimal choice is .....
1: X(i,k,o1,a) < -- ( 1.00000000) D2(i,o3,k,o2) T2(o3,o2,o1,a)
2: S2(i,k,m,a) < -- ( -1.00000000) X(i,k,o1,a) Y13(m,o1)
! Scaling : O(o^5v^1)
! Max size of X : o^3
! * Begin scaling analysis .... *
Declare Y13 as a tensor
for cl in {core}:
 Read V2 from GA for c1
for a in {vir}:
 Read T2 from GA for a
 Read S2 from GA for a
 Declare X as a o^3 tensor
 X_{-}(a)(i,k,o1) += 1.0 sum(o3,o2) D2(i,o3,k,o2) * T2(o3,o2,o1,)
 S2_{(a)}(i,k,m) += -1 sum(o1) X_{(a)}(i,k,o1,) * Y13(m,o1)
 Accumulate S2_(a)(i,k,m) for a
! No.27
```

```
eclipse sort.dat
  9 11, 12 16:46
                                                                   Page 118/145
! S2(i,k,m,a) < --
! ( 0.50000000) D3(i,m,k,o3,o4,o2) T2(o1,o3,o4,a) Y14(o1,o2)
! Indices of BareAmp are rotated to match with LHS.
Case 0 ..... X(i,m,k,o2,o1,a) < ---- (1.00000000) D3(i,m,k,o3,o4,o2) T2(o1
,o3,o4,a)
! Polynomial order is O(o^7v^1)
! Maximum memory usage is O(o^5)
Case 1 ..... X(i,m,k,o3,o4,o1) <---- ( 1.00000000) D3(i,m,k,o3,o4,o2) Y14(
01.02
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^6)
Case 2 ..... X(o3,o4,o2,a) <---- ( 1.00000000) T2(o1,o3,o4,a) Y14(o1,o2)
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^3)
Factorize: Conflict between choices of optimal memory usage and polynomial order
! The optimal choice is .....
1: X(i,m,k,o3,o4,o1) < -- ( 1.00000000) D3(i,m,k,o3,o4,o2) Y14(o1,o2)
2: S2(i,k,m,a) <-- ( 0.50000000) T2(o1,o3,o4,a) X(i,m,k,o3,o4,o1)
! Scaling
             : O(o^6v^1)
! Max size of X : o^6
! * Begin scaling analysis .... *
Declare Y14 as a tensor
for c1 in {core}:
 Read V2 from GA for c1
Declare X as a o^6 tensor
X_{()}(i,m,k,o3,o4,o1) += 1.0 sum(o2) D3(i,m,k,o3,o4,o2) * Y14(o1,o2)
for a in {vir}:
 Read S2 from GA for a
  Read T2 from GA for a
  S2_{(a)}(i,k,m) += 0.5 sum(o1,o3,o4) T2(o1,o3,o4,) * X_{()}(i,m,k,o3,o4,o1)
  Accumulate S2_(a)(i,k,m) for a
1 No. 28
! S2(i,k,m,a) <--
! ( 0.50000000) D2(i,o3,k,o2) T2(o1,o2,m,a) Y15(o1,o3)
! Indices of BareAmp are rotated to match with LHS.
Case 0 .... X(i,o3,k,o1,m,a) <---- ( 1.00000000) D2(i,o3,k,o2) T2(o1,o2,m
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^5)
Case 1 ..... X(i,k,o2,o1) < ---- (1.00000000) D2(i,o3,k,o2) Y15(o1,o3)
! Polynomial order is O(o^5v^1)
! Maximum memory usage is O(o^4)
Case 2 ..... X(0.2, m, 0.3, a) < ---- ( 1.00000000) T2(01, 0.2, m, a) Y15(01, 0.3)
! Polynomial order is O(o^5v^1)
! Maximum memory usage is O(o^3)
Factorize: Conflict between choices of optimal memory usage and polynomial order
! The optimal choice is .....
1: X(i,k,o2,o1) <-- ( 1.00000000) D2(i,o3,k,o2) Y15(o1,o3) 
2: S2(i,k,m,a) <-- ( 0.50000000) T2(o1,o2,m,a) X(i,k,o2,o1)
! Scaling
              : O(o^5v^1)
! Max size of X : o^4
! * Begin scaling analysis .... *
```

```
eclipse_sort.dat
 9 11, 12 16:46
                                                                  Page 119/145
Declare Y15 as a tensor
for c1 in {core}:
 Read V2 from GA for c1
Declare X as a o^4 tensor
X()(i,k,o2,o1) += 1.0 sum(o3) D2(i,o3,k,o2) * Y15(o1,o3)
for a in {vir}:
 Read S2 from GA for a
 Read T2 from GA for a
 S2_{(a)}(i,k,m) += 0.5 sum(o1,o2) T2(o1,o2,m,) * X_{()}(i,k,o2,o1)
 Accumulate S2 (a)(i,k,m) for a
! No.29
! S2(i,k,m,a) <--
! (0.50000000) D3(i,m,k,o3,o4,o2) T2(o2,o1,o4,a) Y16(o1,o3)
! Indices of BareAmp are rotated to match with LHS.
Case 0 .... X(i,m,k,o3,o1,a) <---- ( 1.00000000) D3(i,m,k,o3,o4,o2) T2(o2
! Polynomial order is O(o^7v^1)
! Maximum memory usage is O(o^5)
Case 1 ..... X(i,m,k,o4,o2,o1) < ---- ( 1.00000000) D3(i,m,k,o3,o4,o2) Y16(
01,03)
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^6)
Case 2 ..... X(o2,o4,o3,a) <---- ( 1.00000000) T2(o2,o1,o4,a) Y16(o1,o3)
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^3)
Factorize: Conflict between choices of optimal memory usage and polynomial order
! The optimal choice is .....
1: X(i, m, k, 04, 02, 01) <-- ( 1.00000000) D3(i, m, k, 03, 04, 02) Y16(01, 03)
2: S2(i,k,m,a) < -- ( 0.50000000) T2(o2,o1,o4,a) \times (i,m,k,o4,o2,o1)
! Scaling
             : O(o^6v^1)
! Max size of X : o^6
! * Begin scaling analysis .... *
Declare Y16 as a tensor
for c1 in {core}:
Read V2 from GA for c1
Declare X as a o^6 tensor
X_{()}(i,m,k,o4,o2,o1) += 1.0 sum(o3) D3(i,m,k,o3,o4,o2) * Y16(o1,o3)
for a in {vir}:
Read S2 from GA for a
 Read T2 from GA for a
 S2_{(a)}(i,k,m) += 0.5 \text{ sum}(02,01,04) T2(02,01,04) * X_{()}(i,m,k,04,02,01)
Accumulate S2_(a)(i,k,m) for a
1 No. 30
! S2(i,k,m,a) <--
! ( 0.50000000) D2(i,o3,k,o2) T2(o3,o1,m,a) Y17(o1,o2)
! Indices of BareAmp are rotated to match with LHS.
Case 0 .... X(i,k,o2,o1,m,a) < ---- (1.00000000) D2(i,o3,k,o2) T2(o3,o1,m)
```

```
eclipse sort.dat
  9 11, 12 16:46
                                                                      Page 120/145
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^5)
Case 1 .... X(i,o3,k,o1) < ---- (1.00000000) D2(i,o3,k,o2) Y17(o1,o2)
! Polynomial order is O(o^5v^1)
! Maximum memory usage is O(o^4)
Case 2 ..... X(03,m,02,a) < ---- (1.00000000) T2(03,01,m,a) Y17(01,02)
! Polynomial order is O(o^5v^1)
! Maximum memory usage is O(o^3)
Factorize: Conflict between choices of optimal memory usage and polynomial order
! The optimal choice is .....
1: X(i,03,k,01) < -- ( 1.00000000) D2(i,03,k,02) Y17(01,02) 2: S2(i,k,m,a) < -- ( 0.50000000) T2(03,01,m,a) X(i,03,k,01)
               : O(o^5v^1)
! Max size of X : o^4
! * Begin scaling analysis .... *
Declare Y17 as a tensor
for c1 in {core}:
 Read V2 from GA for c1
Declare X as a o^4 tensor
X_{()}(i,o3,k,o1) += 1.0 sum(o2) D2(i,o3,k,o2) * Y17(o1,o2)
for a in {vir}:
 Read S2 from GA for a
  Read T2 from GA for a
  S2_{(a)}(i,k,m) += 0.5 \text{ sum}(03,01) T2(03,01,m,) * X_{(i)}(i,03,k,01)
  Accumulate S2 (a)(i,k,m) for a
! S2(i,k,m,a) <--
! (0.50000000) D3(k,o2,o3,m,o4,o1) T2(o1,o2,o4,a) Y18(i,o3)
! Indices of BareAmp are rotated to match with LHS.
Case 0 ..... X(k,o3,m,a) < ---- (1.00000000) D3(k,o2,o3,m,o4,o1) T2(o1,o2,
o4,a)
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^3)
Case 1 ..... X(k,o2,m,o4,o1,i) <---- ( 1.00000000) D3(k,o2,o3,m,o4,o1) Y18
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^6)
Case 2 ..... X(o1,o2,o4,i,o3,a) <---- ( 1.00000000) T2(o1,o2,o4,a) Y18(i,o
! Polynomial order is O(o^7v^1)
! Maximum memory usage is O(o^5)
! The optimal choice is .....
1: X(k,03,m,a) <-- ( 1.00000000) D3(k,02,03,m,04,01) T2(01,02,04,a) 
2: S2(i,k,m,a) <-- ( 0.50000000) X(k,03,m,a) Y18(i,03)
! Scaling : O(o^6v^1)
! Max size of X : o^3
! * Begin scaling analysis .... *
Declare Y18 as a tensor
for c1 in {core}:
 Read V2 from GA for c1
```

```
9 11, 12 16:46
                               eclipse sort.dat
                                                                   Page 121/145
for a in {vir}:
 Read T2 from GA for a
 Read S2 from GA for a
 Declare X as a o^3 tensor
 X_{(a)}(k,o3,m) += 1.0 sum(o2,o4,o1) D3(k,o2,o3,m,o4,o1) * T2(o1,o2,o4,)
 S2 (a)(i,k,m) += 0.5 sum(o3) X (a)(k,o3,m,) * Y18(i,o3)
 Accumulate S2 (a)(i,k,m) for a
1 No 32
! S2(i,k,m,a) <--
! ( 0.50000000) D2(k,o2,o3,o1) T2(o1,o2,m,a) Y19(i,o3)
! Indices of BareAmp are rotated to match with LHS.
Case 0 ..... X(k,o3,m,a) < ---- (1.00000000) D2(k,o2,o3,o1) T2(o1,o2,m,a)
! Polynomial order is O(o^5v^1)
! Maximum memory usage is O(o^3)
Case 1 ..... X(k,02,01,i) <---- ( 1.00000000) D2(k,02,03,01) Y19(i,03)
! Polynomial order is O(o^5v^1)
! Maximum memory usage is O(o^4)
Case 2 ..... X(o1,o2,m,i,o3,a) <---- ( 1.00000000) T2(o1,o2,m,a) Y19(i,o3)
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^5)
! The optimal choice is .....
1: X(k,03,m,a) < -- ( 1.00000000) D2(k,02,03,01) T2(01,02,m,a) 2: S2(i,k,m,a) < -- ( 0.50000000) X(k,03,m,a) Y19(i,03)
! Scaling
              : O(o^5v^1)
! Max size of X : o^3
! * Begin scaling analysis .... *
Declare Y19 as a tensor
for cl in {core}:
 Read V2 from GA for cl
for a in {vir}:
 Read T2 from GA for a
 Read S2 from GA for a
 Declare X as a o^3 tensor
 X (a)(k,o3,m) += 1.0 sum(o2,o1) D2(k,o2,o3,o1) * T2(o1,o2,m,)
 S2_{(a)}(i,k,m) += 0.5 sum(o3) X_{(a)}(k,o3,m,) * Y19(i,o3)
 Accumulate S2_(a)(i,k,m) for a
! No.33
! S2(i,k,m,a) <--
! (0.50000000) D3(i,m,o3,o1,o4,o2) T2(o2,o1,o4,a) Y20(k,o3)
! Indices of BareAmp are rotated to match with LHS.
Case 0 .... X(i,m,o3,a) <---- ( 1.00000000) D3(i,m,o3,o1,o4,o2) T2(o2,o1,
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^3)
Case 1 ..... X(i,m,o1,o4,o2,k) <---- ( 1.00000000) D3(i,m,o3,o1,o4,o2) Y20
(k, o3)
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^6)
Case 2 ..... X(02,01,04,k,03,a) < ---- ( 1.00000000) T2(02,01,04,a) Y20(k,o)
```

```
eclipse sort.dat
                                                                    Page 122/145
  9 11, 12 16:46
! Polynomial order is O(o^7v^1)
! Maximum memory usage is O(o^5)
! The optimal choice is .....
1: X(i,m,o3,a) \leftarrow (1.00000000) D3(i,m,o3,o1,o4,o2) T2(o2,o1,o4,a)
2: S2(i,k,m,a) < -- (
                        0.50000000) X(i,m,o3,a) Y20(k,o3)
! Scaling
             : O(o^6v^1)
! Max size of X : o^3
! * Begin scaling analysis .... *
Declare Y20 as a tensor
for c1 in {core}:
 Read V2 from GA for c1
for a in {vir}:
 Read T2 from GA for a
  Read S2 from GA for a
  Declare X as a o^3 tensor
  X (a)(i,m,o3) += 1.0 sum(o1,o4,o2) D3(i,m,o3,o1,o4,o2) * T2(o2,o1,o4,)
  S2_{(a)(i,k,m)} += 0.5 sum(o3) X_{(a)(i,m,o3,)} * Y20(k,o3)
  Accumulate S2_(a)(i,k,m) for a
! No.34
! S2(i,k,m,a) <--
! ( 0.50000000) D2(i,o2,o3,o1) T2(o2,o1,m,a) Y21(k,o3)
! Indices of BareAmp are rotated to match with LHS.
Case 0 ..... X(i,o3,m,a) < ---- ( 1.00000000) D2(i,o2,o3,o1) T2(o2,o1,m,a)
! Polynomial order is O(o^5v^1)
! Maximum memory usage is O(o^3)
Case 1 ..... X(i,o2,o1,k) <---- ( 1.00000000) D2(i,o2,o3,o1) Y21(k,o3)
! Polynomial order is O(o^5v^1)
! Maximum memory usage is O(o^4)
Case 2 ..... X(o2,o1,m,k,o3,a) <---- ( 1.00000000) T2(o2,o1,m,a) Y21(k,o3)
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^5)
! The optimal choice is .....
1: X(i,o3,m,a) <-- ( 1.00000000) D2(i,o2,o3,o1) T2(o2,o1,m,a) 
2: S2(i,k,m,a) <-- ( 0.50000000) X(i,o3,m,a) Y21(k,o3)
! Scaling : O(o^5v^1)
! Max size of X : o^3
! * Begin scaling analysis .... *
Declare Y21 as a tensor
for c1 in {core}:
  Read V2 from GA for c1
for a in {vir}:
  Read T2 from GA for a
  Read S2 from GA for a
  Declare X as a o^3 tensor
  X (a)(i,o3,m) += 1.0 sum(o2,o1) D2(i,o2,o3,o1) * T2(o2,o1,m,)
  S2_{(a)}(i,k,m) += 0.5 sum(o3) X_{(a)}(i,o3,m,) * Y21(k,o3)
  Accumulate S2_(a)(i,k,m) for a
```

```
eclipse sort.dat
 9 11, 12 16:46
                                                                  Page 123/145
! No.35
! S2(i,k,m,a) <--
! (2.00000000) D3(i,m,k,o2,o3,o1) T2(o1,o2,o3,v1) Y22(a,v1)
3,v1)
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^3)
Case 1 ..... X(i,m,k,o2,o3,o1,a,v1) <---- ( 1.00000000) D3(i,m,k,o2,o3,o1)
Y22(a,v1)
! Polynomial order is O(o^6v^2)
! Maximum memory usage is O(o^6)
Case 2 ..... X(o1,o2,o3,a) <---- ( 1.00000000) T2(o1,o2,o3,v1) Y22(a,v1)
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^3)
! The optimal choice is .....
1: X(i,m,k,v1) <-- ( 1.00000000) D3(i,m,k,o2,o3,o1) T2(o1,o2,o3,v1)
2: S2(i,k,m,a) <-- ( 2.00000000) X(i,m,k,v1) Y22(a,v1)
! Scaling : 0(o^6v^1)
! Max size of X : o^3
! * Begin scaling analysis .... *
Declare Y22 as a tensor
for c1 in {core}:
 Read V2 from GA for c1
for v1 in {vir}:
 Read T2 from GA for v1
 Declare X as a o^3 tensor
 X_{(v1)(i,m,k)} += 1.0 \text{ sum}(02,03,01) \text{ D3}(i,m,k,02,03,01) * T2(01,02,03,)
 for a in {vir}:
   Read S2 from GA for a
   S2 (a)(i,k,m) += 2 sum() X (v1)(i,m,k,) * Y22(a,v1)
   Accumulate S2_(a)(i,k,m) for a
! No.36
! S2(i,k,m,a) < --
! ( 2.00000000) D2(i,o2,k,o1) T2(o2,o1,m,v1) Y23(a,v1)
Case 0 ..... X(i,k,m,v1) <---- ( 1.00000000) D2(i,o2,k,o1) T2(o2,o1,m,v1)
! Polynomial order is O(o^5v^1)
! Maximum memory usage is O(o^3)
Case 1 ..... X(i,o2,k,o1,a,v1) < ---- (1.00000000) D2(i,o2,k,o1) Y23(a,v1)
! Polynomial order is O(o^5v^2)
! Maximum memory usage is O(o^4)
Case 2 ..... X(02,01,m,a) < ---- (1.00000000) T2(02,01,m,v1) Y23(a,v1)
! Polynomial order is O(o^5v^1)
! Maximum memory usage is O(o^3)
! The optimal choice is .....
1: X(i,k,m,v1) < -- ( 1.00000000) D2(i,o2,k,o1) T2(o2,o1,m,v1) 2: S2(i,k,m,a) < -- ( 2.00000000) X(i,k,m,v1) Y23(a,v1)
! Scaling
              : O(o^5v^1)
! Max size of X : o^3
! * Begin scaling analysis .... *
```

```
eclipse sort.dat
  9 11, 12 16:46
                                                                   Page 124/145
Declare Y23 as a tensor
for c1 in {core}:
 Read V2 from GA for c1
for v1 in {vir}:
  Read T2 from GA for v1
  Declare X as a o^3 tensor
  X(v1)(i,k,m) += 1.0 sum(o2,o1) D2(i,o2,k,o1) * T2(o2,o1,m,)
  for a in {vir}:
   Read S2 from GA for a
    S2 (a)(i,k,m) += 2 sum() X (v1)(i,k,m,) * Y23(a,v1)
   Accumulate S2_(a)(i,k,m) for a
1 No 37
! S2(i,k,m,a) <--
! ( -1.00000000) D3(i,m,k,o2,o3,o1) T2(o1,o2,o3,v1) Y24(a,v1)
Case 0 \dots X(i,m,k,v1) < ---- (1.00000000) D3(i,m,k,o2,o3,o1) T2(o1,o2,o
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^3)
Case 1 ..... X(i,m,k,o2,o3,o1,a,v1) <---- ( 1.00000000) D3(i,m,k,o2,o3,o1)
Y24(a,v1)
! Polynomial order is O(o^6v^2)
! Maximum memory usage is O(o^6)
Case 2 ..... X(o1,o2,o3,a) < ---- ( 1.00000000) T2(o1,o2,o3,v1) Y24(a,v1)
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^3)
! The optimal choice is .....
1: X(i,m,k,v1) < -- ( 1.00000000) D3(i,m,k,o2,o3,o1) T2(o1,o2,o3,v1) 2: S2(i,k,m,a) < -- ( -1.00000000) X(i,m,k,v1) Y24(a,v1)
! Scaling
              : O(o^6v^1)
! Max size of X : o^3
! * Begin scaling analysis .... *
Declare Y24 as a tensor
for cl in {core}:
 Read V2 from GA for cl
for v1 in {vir}:
  Read T2 from GA for v1
  Declare X as a o^3 tensor
  X (v1)(i,m,k) += 1.0 sum(o2,o3,o1) D3(i,m,k,o2,o3,o1) * T2(o1,o2,o3,)
  for a in {vir}:
   Read S2 from GA for a
    S2_{(a)}(i,k,m) += -1 sum() X_{(v1)}(i,m,k,) * Y24(a,v1)
   Accumulate S2_(a)(i,k,m) for a
! No.38
! S2(i,k,m,a) <--
! (-1.00000000) D2(i,o2,k,o1) T2(o2,o1,m,v1) Y25(a,v1)
Case 0 ..... X(i,k,m,v1) < ---- ( 1.00000000) D2(i,o2,k,o1) T2(o2,o1,m,v1)
! Polynomial order is O(o^5v^1)
! Maximum memory usage is O(o^3)
```

```
eclipse sort.dat
 9 11, 12 16:46
                                                              Page 125/145
Case 1 .... X(i,o2,k,o1,a,v1) < ---- (
                                         1.00000000) D2(i,o2,k,o1) Y25(a,v1)
! Polynomial order is O(o^5v^2)
! Maximum memory usage is O(o^4)
Case 2 ..... X(02,01,m,a) < ---- ( 1.00000000) T2(02,01,m,v1) Y25(a,v1)
! Polynomial order is O(o^5v^1)
! Maximum memory usage is O(o^3)
! The optimal choice is .....
! Scaling : O(o^5v^1)
! Max size of X : o^3
! * Begin scaling analysis .... *
Declare Y25 as a tensor
for c1 in {core}:
 Read V2 from GA for c1
for v1 in {vir}:
 Read T2 from GA for v1
 Declare X as a o^3 tensor
 X(v1)(i,k,m) += 1.0 sum(o2,o1) D2(i,o2,k,o1) * T2(o2,o1,m,)
 for a in {vir}:
   Read S2 from GA for a
   S2_{(a)}(i,k,m) += -1 sum() X_{(v1)}(i,k,m,) * Y25(a,v1)
   Accumulate S2 (a)(i,k,m) for a
! No.39
! S2(i,k,m,a) <--
! ( 0.50000000) D4(i,o4,k,o3,o5,o1,o6,o2) T2(o2,o3,o6,a) V2(m,o4,o1,o5)
! Indices of BareAmp are rotated to match with LHS.
! Indices of ERI and D4 are rotated to match with each other.
H2: 1 D4: 1
*TEST* ( 0.50000000) D4(04,i,03,k,01,05,02,06) T2(02,03,06,a) V2(04,m,01,05)
! *** D4(04,i,03,k,01,05,02,06) T2(02,03,06,a) is skipped due to the priority
Case 1 .... X(i,o3,k,o2,o6,m) <---- ( 1.00000000) D4(o4,i,o3,k,o1,o5,o2,o
6) V2(o4,m,o1,o5)
! Polynomial order is O(o^9)
! Maximum memory usage is O(o^5)
Case 2 ..... X(02.03.06.04.m.01.05.a) <---- ( 1.00000000) T2(02.03.06.a) V
2(o4,m,o1,o5)
! Polynomial order is O(o^9v^1)
! Maximum memory usage is O(o^6)
! The optimal choice is .....
1: X(i,03,k,02,06,m) < -- ( 1.00000000) D4(04,i,03,k,01,05,02,06) V2(04,m,0)
2: S2(i,k,m,a) < -- ( 0.50000000) T2(o2,o3,o6,a) X(i,o3,k,o2,o6,m)
! Scaling
           : O(o^9)
! Max size of X : o^5
! * Begin scaling analysis .... *
! Intermediate is not processed in ad hoc fashion ....
Declare X as a o^6 tensor
for o4 in {occ}:
 Read V2 from GA for o4
 for i in {occ}:
```

```
eclipse sort.dat
  9 11, 12 16:46
                                                                  Page 126/145
    Read D4 from GA for o4,i
    X_{()}(i,03,k,02,06,m) += 1.0 sum(01,05) V2(,m,01,05) * D4(,,03,k,01,05,02,06)
for a in {vir}:
  Read S2 from GA for a
  Read T2 from GA for a
  S2(a)(i,k,m) += 0.5 sum(o2,o3,o6) T2(o2,o3,o6,) * X()(i,o3,k,o2,o6,m)
  Accumulate S2 (a)(i,k,m) for a
! No.40
! S2(i,k,m,a) <--
! ( 0.50000000) D4(i,m,k,o4,o5,o2,o6,o3) T2(o3,o4,o1,a) V2(o1,o6,o2,o5)
! Indices of BareAmp are rotated to match with LHS.
! Indices of ERI and D4 are rotated to match with each other.
H2: 1 D4: 36
*TEST* ( 0.50000000) D4(06,03,i,m,k,04,05,02) T2(03,04,01,a) V2(06,01,02,05)
! *** D4(06,03,i,m,k,04,05,02) T2(03,04,01,a) is skipped due to the priority
Case 1 .... X(03,i,m,k,04,01) < ---- (1.00000000) D4(06,03,i,m,k,04,05,02)
) V2(06,01,02,05)
! Polynomial order is O(o^9)
! Maximum memory usage is O(o^5)
Case 2 ..... X(03,04,06,02,05,a) <---- ( 1.00000000) T2(03,04,01,a) V2(06,
01,02,05)
! Polynomial order is O(o^8v^1)
! Maximum memory usage is O(o^3)
Factorize: Conflict between choices of optimal memory usage and polynomial order
! The optimal choice is .....
1: X(03,i,m,k,04,01) < -- ( 1.00000000) D4(06,03,i,m,k,04,05,02) V2(06,01,0)
2,05)
2: S2(i,k,m,a) < -- ( 0.50000000) T2(03,04,01,a) X(03,i,m,k,04,01)
! Scaling
              : O(o^9)
! Max size of X : o^5
! * Begin scaling analysis .... *
! Intermediate is not processed in ad hoc fashion ....
Declare X as a o^6 tensor
for o6 in {occ}:
 Read V2 from GA for o6
  for o3 in {occ}:
    Read D4 from GA for o6.03
    X_{-}()(03,i,m,k,04,01) += 1.0 sum(02,05) V2(,01,02,05) * D4(,,i,m,k,04,05,02)
for a in {vir}:
 Read S2 from GA for a
  Read T2 from GA for a
  S2_{(a)}(i,k,m) += 0.5 \text{ sum}(03,04,01) T2(03,04,01,) * X_{()}(03,i,m,k,04,01)
 Accumulate S2_(a)(i,k,m) for a
! No.41
! S2(i,k,m,a) <--
! (1.00000000) D3(i,04,k,03,05,02) T2(04,03,01,a) V2(m,01,02,05)
! Indices of BareAmp are rotated to match with LHS.
! *** D3(i,04,k,03,05,02) T2(04,03,01,a) is skipped due to the priority
Case 1 .... X(i,04,k,03,m,01) < ---- (1.00000000) D3(i,04,k,03,05,02) V2(
```

```
9 11, 12 16:46
                                                                                                  eclipse sort.dat
                                                                                                                                                                                                                 Page 127/145
m, o1, o2, o5)
! Polynomial order is O(o^8)
 ! Maximum memory usage is O(o^5)
Case 2 ..... X(04,03,m,02,05,a) < ---- ( 1.00000000) T2(04,03,01,a) V2(m,o1) V2(m,
 ,02,05)
! Polynomial order is O(o^7v^1)
 ! Maximum memory usage is O(o^4)
Factorize: Conflict between choices of optimal memory usage and polynomial order
 ! The optimal choice is .....
1: X(i, 04, k, 03, m, 01) < -- ( 1.00000000) D3(i, 04, k, 03, 05, 02) V2(m, 01, 02, 05)
2: S2(i,k,m,a) < -- ( 1.00000000) T2(04,03,01,a) \times (i,04,k,03,m,01)
 ! Scaling
                                            : O(o^8)
! Max size of X : o^5
! * Begin scaling analysis .... *
for m in {occ}:
     Read V2 from GA for m
      Declare X as a o^5 tensor
     X_{m}(0)(i,04,k,03,01) += 1.0 sum(02,05) V2(,01,02,05) * D3(i,04,k,03,05,02)
     for a in {vir}:
            Read S2 from GA for a
            Read T2 from GA for a
            S2(a)(i,k,m) += 1.0 sum(04,03,01) T2(04,03,01,) * X(m)(i,04,k,03,,01)
            Accumulate S2 (a)(i,k,m) for a
! No.42
! S2(i,k,m,a) <--
! (1.00000000) D3(i,o4,k,o3,o5,o2) T2(o2,o3,o1,a) V2(m,o4,o1,o5)
! Indices of BareAmp are rotated to match with LHS.
! *** D3(i,o4,k,o3,o5,o2) T2(o2,o3,o1,a) is skipped due to the priority Case 1 .... X(i,k,o3,o2,m,o1) <---- ( 1.00000000) D3(i,o4,k,o3,o5,o2) V2(
m, 04, 01, 05)
! Polynomial order is O(o^8)
! Maximum memory usage is O(o^5)
Case 2 ..... X(02,03,m,04,05,a) < ---- ( 1.00000000) T2(02,03,01,a) V2(m,04) T2(m,04) T2(m,04) T2(m,04) T2(m,04) T2(m,04) T2
,01,05)
! Polynomial order is O(o^7v^1)
! Maximum memory usage is O(o^4)
Factorize: Conflict between choices of optimal memory usage and polynomial order
 ! The optimal choice is .....
1: X(i, k, o3, o2, m, o1) <-- ( 1.00000000) D3(i, o4, k, o3, o5, o2) V2(m, o4, o1, o5) 
2: S2(i, k, m, a) <-- ( 1.00000000) T2(o2, o3, o1, a) X(i, k, o3, o2, m, o1)
! Scaling
                                            : O(o^8)
! Max size of X : o^5
! * Begin scaling analysis .... *
for m in {occ}:
     Read V2 from GA for m
     Declare X as a o^5 tensor
     X (m)(i,k,03,02,01) += 1.0 sum(04.05) V2(.04.01.05) * D3(i,04.k,03.05.02)
     for a in {vir}:
           Read S2 from GA for a
             Read T2 from GA for a
            S2_{(a)}(i,k,m) += 1.0 sum(02,03,01) T2(02,03,01,) * X_{(m)}(i,k,03,02,,01)
```

```
eclipse sort.dat
                                                               Page 128/145
 9 11, 12 16:46
   Accumulate S2_(a)(i,k,m) for a
! No.43
! S2(i,k,m,a) < --
! ( -0.50000000) D4(i,m,k,04,05,02,06,03) T2(01,04,06,a) V2(01,03,02,05)
! Indices of BareAmp are rotated to match with LHS.
! Indices of ERI and D4 are rotated to match with each other.
H2: 1 D4: 37
*TEST* ( -0.50000000) D4(03,06,m,i,04,k,02,05) T2(01,04,06,a) V2(03,01,02,05)
! *** D4(03,06,m,i,04,k,02,05) T2(01,04,06,a) is skipped due to the priority
Case 1 ..... X(06,m,i,04,k,01) <---- ( 1.00000000) D4(03,06,m,i,04,k,02,05
) V2(o3,o1,o2,o5)
! Polynomial order is O(o^9)
! Maximum memory usage is O(o^5)
Case 2 ..... X(04,06,03,02,05,a) <---- ( 1.00000000) T2(01,04,06,a) V2(03,
01,02,05)
! Polynomial order is O(o^8v^1)
! Maximum memory usage is O(o^3)
Factorize: Conflict between choices of optimal memory usage and polynomial order
! The optimal choice is .....
2,05)
2: S2(i,k,m,a) < -- ( -0.50000000) T2(o1,o4,o6,a) X(o6,m,i,o4,k,o1)
! Scaling
             : O(o^9)
! Max size of X : o^5
! * Begin scaling analysis .... *
! Intermediate is not processed in ad hoc fashion ....
Declare X as a o^6 tensor
for o3 in {occ}:
 Read V2 from GA for o3
 for o6 in {occ}:
   Read D4 from GA for o3.06
   X_{()}(06,m,i,04,k,01) += 1.0 sum(02,05) V2(,01,02,05) * D4(,,m,i,04,k,02,05)
for a in {vir}:
 Read S2 from GA for a
  Read T2 from GA for a
  S2_{(a)}(i,k,m) += -0.5 \text{ sum}(01,04,06) T2(01,04,06,) * X_{()}(06,m,i,04,k,01)
 Accumulate S2_(a)(i,k,m) for a
! No.44
! S2(i,k,m,a) <--
! (-0.50000000) D3(i,04,k,03,05,02) T2(01,03,m,a) V2(01,04,02,05)
! Indices of BareAmp are rotated to match with LHS.
! *** D3(i,o4,k,o3,o5,o2) T2(o1,o3,m,a) is skipped due to the priority
Case 1 ..... X(i,k,o3,o1) < ---- ( 1.00000000) D3(i,o4,k,o3,o5,o2) V2(o1,o4)
,02,05)
! Polynomial order is O(o^7)
! Maximum memory usage is O(o^3)
Case 2 .... X(03,m,04,02,05,a) <---- ( 1.00000000) T2(01,03,m,a) V2(01,04
,02,05)
! Polynomial order is O(o^7v^1)
! Maximum memory usage is O(o^5)
```

```
eclipse sort.dat
 9 11, 12 16:46
                                                                      Page 129/145
! The optimal choice is .....
1: X(i,k,03,01) < -- ( 1.00000000) D3(i,04,k,03,05,02) V2(01,04,02,05) 2: S2(i,k,m,a) < -- ( -0.50000000) T2(01,03,m,a) X(i,k,03,01)
               : O(0^{7})
! Scaling
! Max size of X : o^3
! * Begin scaling analysis .... *
for ol in {occ}:
 Read V2 from GA for ol
 Declare X as a o^3 tensor
 X(01)(i,k,03) += 1.0 sum(04,02,05) V2(,04,02,05) * D3(i,04,k,03,05,02)
 for a in {vir}:
    Read S2 from GA for a
    Read T2 from GA for a
    S2 (a)(i,k,m) += -0.5 sum(o3) T2(o1,o3,m,) * X (o1)(i,k,o3,)
    Accumulate S2 (a)(i,k,m) for a
! No.45
! S2(i,k,m,a) <--
! (-0.50000000) D3(i,04,k,03,05,02) T2(01,03,05,a) V2(m,04,01,02)
! Indices of BareAmp are rotated to match with LHS.
! *** D3(i,o4,k,o3,o5,o2) T2(o1,o3,o5,a) is skipped due to the priority
Case 1 ..... X(i,k,o3,o5,m,o1) <---- ( 1.00000000) D3(i,o4,k,o3,o5,o2) V2(i,o4,b,o3,o5,o2)
m, o4, o1, o2)
! Polynomial order is O(o^8)
! Maximum memory usage is O(o^5)
Case 2 ..... X(03,05,m,04,02,a) <---- ( 1.00000000) T2(01,03,05,a) V2(m,04
,01,02)
! Polynomial order is O(o^7v^1)
! Maximum memory usage is O(o^4)
Factorize: Conflict between choices of optimal memory usage and polynomial order
! The optimal choice is ..... 
 1: X(i,k,o3,o5,m,o1) <-- ( 1.00000000) D3(i,o4,k,o3,o5,o2) V2(m,o4,o1,o2)
2: S2(i,k,m,a) < -- ( -0.50000000) T2(01,03,05,a) X(i,k,03,05,m,01)
! Scaling
             : O(o^8)
! Max size of X : o^5
! * Begin scaling analysis .... *
for m in {occ}:
 Read V2 from GA for m
 Declare X as a o^5 tensor
 X_{m}(m)(i,k,o3,o5,o1) += 1.0 sum(o4,o2) V2(,o4,o1,o2) * D3(i,o4,k,o3,o5,o2)
 for a in {vir}:
    Read S2 from GA for a
    Read T2 from GA for a
    S2_{(a)}(i,k,m) += -0.5 \text{ sum}(01,03,05) T2(01,03,05,) * X_{(m)}(i,k,03,05,,01)
    Accumulate S2_(a)(i,k,m) for a
! No.46
! S2(i,k,m,a) <--
```

```
eclipse sort.dat
    9 11, 12 16:46
                                                                                                                                Page 130/145
 ! (-0.50000000) D4(i,m,k,04,05,02,06,03) T2(03,01,06,a) V2(01,04,02,05)
! Indices of BareAmp are rotated to match with LHS.
 ! Indices of ERI and D4 are rotated to match with each other.
H2: 1 D4: 13
*TEST* ( -0.50000000) D4(04,k,m,i,o2,o5,o3,o6) T2(03,o1,o6,a) V2(04,o1,o2,o5)
! *** D4(04,k,m,i,o2,o5,o3,o6) T2(03,o1,o6,a) is skipped due to the priority
Case 1 ..... X(k,m,i,o3,o6,o1) < ---- (1.00000000) D4(o4,k,m,i,o2,o5,o3,o6)
) V2(o4,o1,o2,o5)
! Polynomial order is O(o^9)
 ! Maximum memory usage is O(o^5)
Case 2 ..... X(03,06,04,02,05,a) <---- ( 1.00000000) T2(03,01,06,a) V2(04,
01,02,05)
! Polynomial order is O(o^8v^1)
! Maximum memory usage is O(o^4)
Factorize: Conflict between choices of optimal memory usage and polynomial order
! The optimal choice is .....
1: X(k,m,i,03,06,01) < -- ( 1.00000000) D4(04,k,m,i,02,05,03,06) V2(04,01,0)
2,05)
2: S2(i,k,m,a) < -- (-0.50000000) T2(03,01,06,a) X(k,m,i,03,06,01)
! Scaling : O(o^9)
! Max size of X : o^5
! * Begin scaling analysis .... *
 ! Intermediate is not processed in ad hoc fashion ....
Declare X as a o^6 tensor
for o4 in {occ}:
  Read V2 from GA for o4
    for k in {occ}:
       Read D4 from GA for o4,k
       X()(k,m,i,o3,o6,o1) += 1.0 sum(o2,o5) V2(,o1,o2,o5) * D4(,,m,i,o2,o5,o3,o6)
for a in {vir}:
    Read S2 from GA for a
    Read T2 from GA for a
    S2(a)(i,k,m) += -0.5 sum(03.01.06) T2(03.01.06.) * X()(k,m,i,03.06.01)
    Accumulate S2_(a)(i,k,m) for a
! No.47
! S2(i,k,m,a) <--
! (-0.50000000) D3(i,04,k,03,05,02) T2(04,01,m,a) V2(01,03,02,05)
! Indices of BareAmp are rotated to match with LHS.
 ! *** D3(i,o4,k,o3,o5,o2) T2(o4,o1,m,a) is skipped due to the priority
Case 1 ..... X(i,04,k,01) < ---- ( 1.00000000) D3(i,04,k,03,05,02) V2(01,03) V2(01,03) V3(01,04,k,03,05,02) V3(01,03,05,03) V3(01,04,k,03,05,02) V3(01,03,05,03) V3(01,04,k,03,05,03) V3(01,04,k,03,05,05,05) V3(01,04,k,03,05,05) V3(01,04,k,03,05,05) V3(01,04,k,05,05) V3(01,04,k,05) V3(01,04,k,05)
,02,05)
! Polynomial order is O(o^7)
! Maximum memory usage is O(o^3)
Case 2 ..... X(04,m,03,02,05,a) < ---- ( 1.00000000) T2(04,01,m,a) V2(01,03)
 ,02,05)
 ! Polynomial order is O(o^7v^1)
! Maximum memory usage is O(o^5)
! The optimal choice is .....
1: X(i,04,k,01) <-- ( 1.00000000) D3(i,04,k,03,05,02) V2(o1,03,02,05) 
2: S2(i,k,m,a) <-- ( -0.50000000) T2(o4,01,m,a) X(i,04,k,01)
! Scaling
                           : O(o^7)
! Max size of X : o^3
 ! * Begin scaling analysis .... *
```

```
eclipse sort.dat
 9 11, 12 16:46
                                                                   Page 131/145
for ol in {occ}:
 Read V2 from GA for ol
 Declare X as a o^3 tensor
 X_{(01)(i,04,k)} += 1.0 \text{ sum}(03,02,05) \text{ V2}(,03,02,05) * D3(i,04,k,03,05,02)
 for a in {vir}:
   Read S2 from GA for a
    Read T2 from GA for a
    S2(a)(i,k,m) += -0.5 sum(o4) T2(o4,o1,m,) * X(o1)(i,o4,k,)
   Accumulate S2_(a)(i,k,m) for a
1 No 48
! S2(i,k,m,a) <--
! ( -0.50000000) D3(i,o4,k,o3,o5,o2) T2(o2,o1,o5,a) V2(m,o4,o1,o3)
! Indices of BareAmp are rotated to match with LHS.
! *** D3(i,o4,k,o3,\bar{o5},o2) T2(o2,o1,o5,a) is skipped due to the priority
Case 1 ..... X(i,k,o5,o2,m,o1) <---- ( 1.00000000) D3(i,o4,k,o3,o5,o2) V2(
m, o4, o1, o3)
! Polynomial order is O(o^8)
! Maximum memory usage is O(o^5)
Case 2 ..... X(0.05,m.04,03,a) <---- ( 1.00000000) T2(0.01,05,a) V2(m.04,03,a)
,01,03)
! Polynomial order is O(o^7v^1)
! Maximum memory usage is O(o^4)
Factorize: Conflict between choices of optimal memory usage and polynomial order
! The optimal choice is ..... 
 1: X(i,k,o5,o2,m,o1) <-- ( 1.00000000) D3(i,o4,k,o3,o5,o2) V2(m,o4,o1,o3)
2: S2(i,k,m,a) < -- ( -0.50000000) T2(o2,o1,o5,a) X(i,k,o5,o2,m,o1)
! Scaling
              : O(o^8)
! Max size of X : o^5
! * Begin scaling analysis .... *
for m in {occ}:
 Read V2 from GA for m
 Declare X as a o^5 tensor
 X (m)(i,k,05,02,01) += 1.0 sum(04,03) V2(.04,01,03) * D3(i,04,k,03,05,02)
 for a in {vir}:
   Read S2 from GA for a
    Read T2 from GA for a
   S2_{(a)}(i,k,m) += -0.5 sum(02,01,05) T2(02,01,05,) * X_{(m)}(i,k,05,02,01)
   Accumulate S2_(a)(i,k,m) for a
! No.49
! S2(i,k,m,a) <--
! ( -0.50000000) D3(i,m,k,o4,o5,o3) T2(o2,o1,o5,a) V2(o1,o4,o2,o3)
! Indices of BareAmp are rotated to match with LHS.
! *** D3(i,m,k,o4,o5,o3) T2(o2,o1,o5,a) is skipped due to the priority
Case 1 .... X(i,m,k,o5,o1,o2) < ---- (1.00000000) D3(i,m,k,o4,o5,o3) V2(o)
1,04,02,03)
! Polynomial order is O(o^8)
! Maximum memory usage is O(o^5)
Case 2 ..... X(05,04,03,a) < ---- (1.00000000) T2(02,01,05,a) V2(01,04,02,a)
```

```
eclipse sort.dat
  9 11, 12 16:46
                                                                         Page 132/145
 ! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^3)
 ! The optimal choice is .....
1: X(05,04,03,a) < -- ( 1.00000000) T2(02,01,05,a) V2(01,04,02,03) 2: S2(i,k,m,a) < -- ( -0.50000000) D3(i,m,k,04,05,03) X(05,04,03,a)
                : O(o^6v^1)
! Scaling
! Max size of X : o^3
! * Begin scaling analysis .... *
! Intermediate is not processed in ad hoc fashion ....
Declare X as a o^3v^1 tensor
for o1 in {occ}:
  Read V2 from GA for o1
  for a in {vir}:
    Read T2 from GA for a
    X_{()}(05,04,03,a) += 1.0 sum(02) V2(,04,02,03) * T2(02,01,05,)
for a in {vir}:
  Read S2 from GA for a
  S2_{(a)}(i,k,m) += -0.5 sum(04,05,03) D3(i,m,k,04,05,03) * X_{()}(05,04,03,a)
  Accumulate S2_(a)(i,k,m) for a
! S2(i,k,m,a) <--
! ( -0.50000000) D2(i,o4,k,o3) T2(o2,o1,m,a) V2(o1,o3,o2,o4)
! Indices of BareAmp are rotated to match with LHS.
! *** D2(i,o4,k,o3) T2(o2,o1,m,a) is skipped due to the priority
Case 1 .... X(i,k,o1,o2) <---- ( 1.00000000) D2(i,o4,k,o3) V2(o1,o3,o2,o4
! Polynomial order is O(o^5v^1)
! Maximum memory usage is O(o^3)
Case 2 ..... X(m,o3,o4,a) < ---- ( 1.00000000) T2(o2,o1,m,a) V2(o1,o3,o2,o4)
! Polynomial order is O(o^5v^1)
! Maximum memory usage is O(o^3)
! The optimal choice is .....
1: X(i,k,o1,o2) <-- ( 1.00000000) D2(i,o4,k,o3) V2(o1,o3,o2,o4)
2: S2(i,k,m,a) <-- ( -0.50000000) T2(o2,o1,m,a) X(i,k,o1,o2)
! Scaling
              : O(o^5v^1)
! Max size of X : o^3
! * Begin scaling analysis .... *
for o1 in {occ}:
  Read V2 from GA for ol
  Declare X as a o^3 tensor
  X_{(01)}(i,k,02) += 1.0 sum(03,04) V2(,03,02,04) * D2(i,04,k,03)
  for a in {vir}:
    Read S2 from GA for a
    Read T2 from GA for a
    S2_{(a)}(i,k,m) += -0.5 \text{ sum}(02) T2(02,01,m,) * X_{(01)}(i,k,02)
    Accumulate S2_(a)(i,k,m) for a
```

```
eclipse sort.dat
 9 11, 12 16:46
                                                                  Page 133/145
! No.51
! S2(i,k,m,a) <--
! (-0.50000000) D4(k,03,04,01,05,m,06,02) T2(02,03,06,a) V2(i,05,01,04)
! Indices of BareAmp are rotated to match with LHS.
! Indices of ERI and D4 are rotated to match with each other.
H2: 1 D4: 24
*TEST* ( -0.50000000) D4(05,m,k,03,04,01,06,02) T2(02,03,06,a) V2(05,i,01,04)
! *** D4(05,m,k,03,04,01,06,02) T2(02,03,06,a) is skipped due to the priority
Case 1 .... X(m,k,03,06,02,i) <---- ( 1.00000000) D4(05,m,k,03,04,01,06,0
2) V2(o5,i,o1,o4)
! Polynomial order is O(o^9)
! Maximum memory usage is O(o^5)
Case 2 ..... X(02,03,06,05,i,01,04,a) < ---- ( 1.00000000) T2(02,03,06,a) V
2(05,i,01,04)
! Polynomial order is O(o^9v^1)
! Maximum memory usage is O(o^6)
! The optimal choice is .....
1: X(m,k,03,06,02,i) < -- ( 1.00000000) D4(05,m,k,03,04,01,06,02) V2(05,i,0)
1,04)
2: S2(i,k,m,a) < -- ( -0.50000000) T2(o2,o3,o6,a) X(m,k,o3,o6,o2,i)
! Scaling
            : O(o^9)
! Max size of X : o^5
! * Begin scaling analysis .... *
! Intermediate is not processed in ad hoc fashion ....
Declare X as a o^6 tensor
for o5 in {occ}:
 Read V2 from GA for o5
 for m in {occ}:
    Read D4 from GA for o5,m
   X_{()}(m,k,03,06,02,i) += 1.0 sum(01,04) V2(,i,01,04) * D4(,,k,03,04,01,06,02)
 Read S2 from GA for a
 Read T2 from GA for a
 S2_{(a)}(i,k,m) += -0.5 \text{ sum}(02,03,06) T2(02,03,06,) * X_{()}(m,k,03,06,02,i)
 Accumulate S2 (a)(i,k,m) for a
! No.52
! S2(i,k,m,a) <--
! ( -0.50000000) D3(k,o3,o4,o1,o5,o2) T2(o2,o3,m,a) V2(i,o5,o1,o4)
! Indices of BareAmp are rotated to match with LHS.
! *** D3(k,o3,o4,o1,o5,o2) T2(o2,o3,m,a) is skipped due to the priority
Case 1 .... X(k,03,02,i) <---- ( 1.00000000) D3(k,03,04,01,05,02) V2(i,05,03,04,01,05,02)
,01,04)
! Polynomial order is O(o^7)
! Maximum memory usage is O(o^3)
Case 2 ..... X(02,03,m,i,05,01,04,a) < ---- ( 1.00000000) T2(02,03,m,a) V2(
i, o5, o1, o4)
! Polynomial order is O(o^8v^1)
! Maximum memory usage is O(o^6)
! The optimal choice is .....
1: \ \bar{X(k,o3,o2,i)} \ <-- \ ( \ 1.00000000) \ D3(k,o3,o4,o1,o5,o2) \ V2(i,o5,o1,o4)
2: S2(i,k,m,a) < -- (-0.50000000) T2(o2,o3,m,a) X(k,o3,o2,i)
! Scaling
              : O(o^7)
! Max size of X : o^3
```

```
eclipse sort.dat
  9 11, 12 16:46
                                                                  Page 134/145
! * Begin scaling analysis .... *
for i in {occ}:
  Read V2 from GA for i
  Declare X as a o^3 tensor
  X(i)(k,03,02) += 1.0 \text{ sum}(05,01,04) V2(,05,01,04) * D3(k,03,04,01,05,02)
  for a in {vir}:
   Read S2 from GA for a
    Read T2 from GA for a
    S2_{(a)}(i,k,m) += -0.5 \text{ sum}(02,03) T2(02,03,m,) * X_{(i)}(k,03,02,)
    Accumulate S2 (a)(i,k,m) for a
! S2(i,k,m,a) <--
! ( -0.50000000) D3(k,o3,o4,o2,o5,m) T2(o2,o3,o1,a) V2(i,o5,o1,o4)
! Indices of BareAmp are rotated to match with LHS.
! *** D3(k,o3,o4,o2,o5,m) T2(o2,o3,o1,a) is skipped due to the priority
Case 1 ..... X(k,03,02,m,i,01) < ---- ( 1.00000000) D3(k,03,04,02,05,m) V2(
i,05,01,04)
! Polynomial order is O(o^8)
! Maximum memory usage is O(o^5)
Case 2 ..... X(02,03,i,05,04,a) < ---- ( 1.00000000) T2(02,03,01,a) V2(i,05)
,01,04)
! Polynomial order is O(o^7v^1)
! Maximum memory usage is O(o^4)
Factorize: Conflict between choices of optimal memory usage and polynomial order
! The optimal choice is .....
1: X(k,03,02,m,i,01) < -- ( 1.00000000) D3(k,03,04,02,05,m) V2(i,05,01,04)
2: S2(i,k,m,a) < -- ( -0.50000000) T2(o2,o3,o1,a) X(k,o3,o2,m,i,o1)
! Scaling
              : O(o^8)
! Max size of X : o^5
! * Begin scaling analysis .... *
for i in {occ}:
 Read V2 from GA for i
  Declare X as a o^5 tensor
  X(i)(k,03,02,m,01) += 1.0 sum(05,04) V2(.05,01,04) * D3(k,03,04,02,05,m)
  for a in {vir}:
   Read S2 from GA for a
    Read T2 from GA for a
    S2_{(a)}(i,k,m) += -0.5 sum(o2,o3,o1) T2(o2,o3,o1,) * X_{(i)}(k,o3,o2,m,,o1)
   Accumulate S2_(a)(i,k,m) for a
! No.54
! S2(i,k,m,a) <--
[ ( -0.50000000) D4(i,m,o4,o1,o5,o2,o6,o3) T2(o3,o2,o6,a) V2(k,o5,o1,o4) ]
! Indices of BareAmp are rotated to match with LHS.
! Indices of ERI and D4 are rotated to match with each other.
H2: 1 D4: 24
*TEST* ( -0.50000000) D4(05,02,i,m,04,01,06,03) T2(03,02,06,a) V2(05,k,01,04)
! *** D4(05,02,i,m,04,01,06,03) T2(03,02,06,a) is skipped due to the priority
Case 1 .... X(02,i,m,06,03,k) < ---- ( 1.00000000) D4(05,02,i,m,04,01,06,0)
3) V2(o5,k,o1,o4)
```

```
eclipse sort.dat
 9 11, 12 16:46
                                                                  Page 135/145
! Polynomial order is O(o^9)
! Maximum memory usage is O(o^5)
Case 2 ..... X(03,02,06,05,k,01,04,a) <---- ( 1.00000000) T2(03,02,06,a) V
2(o5,k,o1,o4)
! Polynomial order is O(o^9v^1)
! Maximum memory usage is O(o^5)
! The optimal choice is .....
2: S2(i,k,m,a) < -- ( -0.50000000) T2(o3,o2,o6,a) X(o2,i,m,o6,o3,k)
! Scaling : 0(o^9)
! Max size of X : o^5
! * Begin scaling analysis .... *
! Intermediate is not processed in ad hoc fashion ....
Declare X as a o^6 tensor
for o5 in {occ}:
 Read V2 from GA for o5
 for o2 in {occ}:
   Read D4 from GA for o5,02
   X_{()}(0.02,i,m,0.6,0.3,k) += 1.0 sum(0.1,0.4) V2(,k,0.1,0.4) * D4(,,i,m,0.4,0.1,0.6,0.3)
for a in {vir}:
 Read S2 from GA for a
 Read T2 from GA for a
 S2_{(a)}(i,k,m) += -0.5 \text{ sum}(03,02,06) T2(03,02,06,) * X_{()}(02,i,m,06,03,k)
 Accumulate S2_(a)(i,k,m) for a
! S2(i,k,m,a) <--
! (-0.50000000) D3(i,03,04,01,05,02) T2(03,02,m,a) V2(k,05,01,04)
! Indices of BareAmp are rotated to match with LHS.
! *** D3(i,o3,o4,o1,o5,o2) T2(o3,o2,m,a) is skipped due to the priority
Case 1 .... X(i,03,02,k) < ---- ( 1.00000000) D3(i,03,04,01,05,02) V2(k,05) 
,01,04)
! Polynomial order is O(o^7)
! Maximum memory usage is O(o^3)
Case 2 ..... X(03,02,m,k,05,01,04,a) <---- ( 1.00000000) T2(03,02,m,a) V2(
k,o5,o1,o4)
! Polynomial order is O(o^8v^1)
! Maximum memory usage is O(o^6)
! The optimal choice is .....
1: X(i,03,02,k) <-- ( 1.00000000) D3(i,03,04,01,05,02) V2(k,05,01,04) 
2: S2(i,k,m,a) <-- ( -0.50000000) T2(03,02,m,a) X(i,03,02,k)
! Scaling
             : O(o^7)
! Max size of X : o^3
! * Begin scaling analysis .... *
for k in {occ}:
 Read V2 from GA for k
 Declare X as a o^3 tensor
 X(k)(i.o3.o2) += 1.0 sum(o5.o1.o4) V2(.o5.o1.o4) * D3(i.o3.o4.o1.o5.o2)
 for a in {vir}:
   Read S2 from GA for a
    Read T2 from GA for a
   S2_{(a)}(i,k,m) += -0.5 \text{ sum}(03,02) T2(03,02,m,) * X_{(k)}(i,03,02,)
```

```
eclipse sort.dat
                                                                    Page 136/145
  9 11, 12 16:46
    Accumulate S2_(a)(i,k,m) for a
! No.56
! S2(i,k,m,a) <--
! ( -0.50000000) D3(i,m,o4,o2,o5,o3) T2(o2,o3,o1,a) V2(k,o5,o1,o4)
! Indices of BareAmp are rotated to match with LHS.
! *** D3(i,m,o4,o2,o5,o3) T2(o2,o3,o1,a) is skipped due to the priority
Case 1 ..... X(i,m,o2,o3,k,o1) < ---- (1.00000000) D3(i,m,o4,o2,o5,o3) V2(
k, o5, o1, o4)
! Polynomial order is O(o^8)
! Maximum memory usage is O(o^5)
Case 2 ..... X(02,03,k,05,04,a) <---- ( 1.00000000) T2(02,03,01,a) V2(k,05,04,a)
,01,04)
! Polynomial order is O(o^7v^1)
! Maximum memory usage is O(o^4)
Factorize: Conflict between choices of optimal memory usage and polynomial order
! The optimal choice is .....
1: X(i,m,o2,o3,k,o1) < -- ( 1.00000000) D3(i,m,o4,o2,o5,o3) V2(k,o5,o1,o4)
2: S2(i,k,m,a) < -- ( -0.50000000) T2(o2,o3,o1,a) X(i,m,o2,o3,k,o1)
! Scaling
               : O(o^8)
! Max size of X : o^5
! * Begin scaling analysis .... *
for k in {occ}:
 Read V2 from GA for k
  Declare X as a o^5 tensor
  X_{(k)(i,m,o2,o3,o1)} += 1.0 \text{ sum}(o5,o4) V2(,o5,o1,o4) * D3(i,m,o4,o2,o5,o3)
  for a in {vir}:
    Read S2 from GA for a
    Read T2 from GA for a
    S2_{(a)}(i,k,m) += -0.5 \text{ sum}(02,03,01) T2(02,03,01,) * X_{(k)}(i,m,02,03,,01)
   Accumulate S2_(a)(i,k,m) for a
! S2(i,k,m,a) <--
! ( -0.50000000) D3(m,o3,o4,o1,o5,o2) T2(o5,o4,o2,a) V2(i,o3,k,o1)
! Indices of BareAmp are rotated to match with LHS.
! *** D3(m,o3,o4,o1,o5,o2) T2(o5,o4,o2,a) is skipped due to the priority
Case 1 .... X(m,o4,o5,o2,i,k) <---- ( 1.00000000) D3(m,o3,o4,o1,o5,o2) V2
(i,o3,k,o1)
! Polynomial order is O(o^8)
! Maximum memory usage is O(o^5)
Case 2 ..... X(05,04,02,i,03,k,01,a) <---- ( 1.00000000) T2(05,04,02,a) V2
(i,o3,k,o1)
! Polynomial order is O(o^8v^1)
! Maximum memory usage is O(o^6)
! The optimal choice is .....
1: X(m,o4,o5,o2,i,k) <-- ( 1.00000000) D3(m,o3,o4,o1,o5,o2) V2(i,o3,k,o1) 2: S2(i,k,m,a) <-- ( -0.50000000) T2(o5,o4,o2,a) X(m,o4,o5,o2,i,k)
! Scaling
              : O(o^8)
! Max size of X : o^5
```

```
eclipse sort.dat
                                                                    Page 137/145
 9 11, 12 16:46
! * Begin scaling analysis .... *
for i in {occ}:
 Read V2 from GA for i
 Declare X as a o^5 tensor
 X_{(i)}(m,04,05,02,k) += 1.0 sum(03,01) V2(,03,k,01) * D3(m,03,04,01,05,02)
 for a in {vir}:
   Read S2 from GA for a
    Read T2 from GA for a
    S2(a)(i,k,m) += -0.5 sum(05,04,02) T2(05,04,02,) * X(i)(m,04,05,02,k)
    Accumulate S2 (a)(i,k,m) for a
! No.58
! S2(i,k,m,a) <--
! ( -0.50000000) D2(o1,o3,o2,o4) T2(o4,o3,m,a) V2(i,o2,k,o1)
! Indices of BareAmp are rotated to match with LHS.
! *** D2(01,03,02,04) T2(04,03,m,a) is skipped due to the priority
Case 1 .... X(03,04,i,k) < ---- ( 1.00000000) D2(01,03,02,04) V2(i,02,k,01) 
! Polynomial order is O(o^5v^1)
! Maximum memory usage is O(o^3)
Case 2 ..... X(04,03,m,i,02,k,01,a) < ---- ( 1.00000000) T2(04,03,m,a) V2(i)
,o2,k,o1)
! Polynomial order is O(o^7v^1)
! Maximum memory usage is O(o^6)
! The optimal choice is .....
1: X(o3,o4,i,k) < -- ( 1.00000000) D2(o1,o3,o2,o4) V2(i,o2,k,o1) 2: S2(i,k,m,a) < -- ( -0.50000000) T2(o4,o3,m,a) X(o3,o4,i,k)
! Scaling
             : O(o^5v^1)
! Max size of X : o^3
! * Begin scaling analysis .... *
for i in {occ}:
 Read V2 from GA for i
 Declare X as a o^3 tensor
 X_{(i)}(03,04,k) += 1.0 \text{ sum}(02,01) V2(,02,k,01) * D2(01,03,02,04)
 for a in {vir}:
   Read S2 from GA for a
    Read T2 from GA for a
    S2_{(a)}(i,k,m) += -0.5 \text{ sum}(04,03) T2(04,03,m,) * X_{(i)}(03,04,k)
   Accumulate S2_(a)(i,k,m) for a
! No.59
! S2(i,k,m,a) <--
! ( 1.0000000) D4(i,m,k,o3,o1,o4,o2,o5) T2(o4,o3,o1,v1) V2(o2,o5,a,v1)
! Indices of ERI are rotated to match with LHS.
! *** D4(i,m,k,o3,o1,o4,o2,o5) T2(o4,o3,o1,v1) is skipped due to the priority
Case 1 .... X(i,m,k,o3,o1,o4,a,v1) < ---- ( 1.00000000) D4(i,m,k,o3,o1,o4,a,v1)
o2.o5) V2(a.v1.o2.o5)
! Polynomial order is O(o^8v^2)
! Maximum memory usage is O(o^4)
Case 2 ..... X(04,03,01,02,05,a) <---- ( 1.00000000) T2(04,03,01,v1) V2(a,
v1,o2,o5)
! Polynomial order is O(o^8v^1)
```

```
9 11, 12 16:46
                               eclipse sort.dat
                                                                  Page 138/145
! Maximum memory usage is O(o^5)
Factorize: Conflict between choices of optimal memory usage and polynomial order
! The optimal choice is .....
1: X(04,03,01,02,05,a) < -- ( 1.00000000) T2(04,03,01,v1) V2(a,v1,02,05)
! Scaling
             : O(o^8v^1)
! Max size of X : o^5
! * Begin scaling analysis .... *
for a in {vir}:
 Read V2 from GA for a
  Read S2 from GA for a
  Declare X as a o^5 tensor
  for v1 in {vir}:
   Read T2 from GA for v1
   X (a)(04,03,01,02,05) += 1.0 sum() V2(,v1,02,05) * T2(04,03,01,)
  for i in {occ}
   for m in {occ}
      Read D4 from GA for i,m
      S2_{(a)}(i,k,m) += 1.0 sum(o3,o1,o4,o2,o5) D4(,,k,o3,o1,o4,o2,o5) * X_{(a)}(o4,o4,o2,o5)
,03,01,02,05,)
      Accumulate S2_(a)(i,k,m) for a
! No.60
! S2(i,k,m,a) <--
! ( 1.00000000) D3(i,o3,k,o2,o4,o1) T2(o3,o2,m,v1) V2(o1,o4,a,v1)
! Indices of ERI are rotated to match with LHS.
! *** D3(i,o3,k,o2,o4,o1) T2(o3,o2,m,v1) is skipped due to the priority
Case 1 .... X(i,o3,k,o2,a,v1) < ---- (1.00000000) D3(i,o3,k,o2,o4,o1) V2(
a,v1,o1,o4)
! Polynomial order is O(o^6v^2)
! Maximum memory usage is O(o^4)
Case 2 ..... X(03,02,m,01,04,a) < ---- ( 1.00000000) T2(03,02,m,v1) V2(a,v1)
,01,04)
! Polynomial order is O(o^7v^1)
! Maximum memory usage is O(o^5)
Factorize: Conflict between choices of optimal memory usage and polynomial order
! The optimal choice is .....
1: X(o3,o2,m,o1,o4,a) <-- ( 1.00000000) T2(o3,o2,m,v1) V2(a,v1,o1,o4) 
2: S2(i,k,m,a) <-- ( 1.00000000) D3(i,o3,k,o2,o4,o1) X(o3,o2,m,o1,o4,a)
! Scaling
              : O(o^7v^1)
! Max size of X : o^5
! * Begin scaling analysis .... *
for a in {vir}:
  Read V2 from GA for a
  Read S2 from GA for a
  Declare X as a o^5 tensor
  for v1 in {vir}:
   Read T2 from GA for v1
   X_{(a)}(03,02,m,01,04) += 1.0 sum() V2(,v1,01,04) * T2(03,02,m,)
  S2_{(a)}(i,k,m) += 1.0 sum(03,02,04,01) D3(i,03,k,02,04,01) * X_{(a)}(03,02,m,01,0)
4,)
```

```
eclipse_sort.dat
 9 11, 12 16:46
                                                                   Page 139/145
 Accumulate S2_(a)(i,k,m) for a
! No.61
! S2(i,k,m,a) <--
! (1.00000000) D3(i,o2,k,o3,o1,o4) T2(o4,o3,o1,v1) V2(m,o2,a,v1)
! Indices of ERI are rotated to match with LHS.
! *** D3(i,o2,k,o3,o1,o4) T2(o4,o3,o1,v1) is skipped due to the priority
Case 1 ..... X(i,k,o3,o1,o4,m,a,v1) < ---- ( 1.00000000) D3(i,o2,k,o3,o1,o4)
) V2(a,v1,m,o2)
! Polynomial order is O(o^7v^2)
! Maximum memory usage is O(o^6)
Case 2 ..... X(04,03,01,m,02,a) < ---- ( 1.00000000) T2(04,03,01,v1) V2(a,v)
1,m,o2)
! Polynomial order is O(o^7v^1)
! Maximum memory usage is O(o^5)
! The optimal choice is .....
1: X(04,03,01,m,02,a) < -- (1.00000000) T2(04,03,01,v1) V2(a,v1,m,02)
2: S2(i,k,m,a) <-- ( 1.00000000) D3(i,o2,k,o3,o1,o4) X(o4,o3,o1,m,o2,a)
! Scaling
             : O(o^7v^1)
! Max size of X : o^5
! * Begin scaling analysis .... *
for a in {vir}:
 Read V2 from GA for a
 Read S2 from GA for a
 Declare X as a o^5 tensor
 for v1 in {vir}:
   Read T2 from GA for v1
   X (a)(04,03,01,m,02) += 1.0 sum() V2(,v1,m,02) * T2(04,03,01,)
 S2_{(a)}(i,k,m) += 1.0 \text{ sum}(02,03,01,04) D3(i,02,k,03,01,04) * X_{(a)}(04,03,01,m,0)
2,)
 Accumulate S2_(a)(i,k,m) for a
! No.62
! S2(i,k,m,a) <--
! ( 1.00000000) D3(i,m,k,o2,o1,o3) T2(o3,o2,o4,v1) V2(o1,o4,a,v1)
! Indices of ERI are rotated to match with LHS.
! *** D3(i,m,k,o2,o1,o3) T2(o3,o2,o4,v1) is skipped due to the priority
Case 1 ..... X(i,m,k,o2,o3,o4,a,v1) < ---- ( 1.00000000) D3(i,m,k,o2,o1,o3)
V2(a,v1,o1,o4)
! Polynomial order is O(o^7v^2)
! Maximum memory usage is O(o^6)
Case 2 ..... X(03,02,01,a) <---- ( 1.00000000) T2(03,02,04,v1) V2(a,v1,01,
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^3)
! The optimal choice is .....
1: X(03,02,01,a) < -- ( 1.00000000) T2(03,02,04,v1) V2(a,v1,01,04) 2: S2(i,k,m,a) < -- ( 1.00000000) D3(i,m,k,02,01,03) X(03,02,01,a)
! Scaling
              : O(o^6v^1)
! Max size of X : o^3
! * Begin scaling analysis .... *
```

```
eclipse sort.dat
  9 11, 12 16:46
                                                                      Page 140/145
for a in {vir}:
  Read V2 from GA for a
  Read S2 from GA for a
  Declare X as a o^3 tensor
  for v1 in {vir}:
   Read T2 from GA for v1
    X_{(a)}(03,02,01) += 1.0 sum(04) V2(,v1,01,04) * T2(03,02,04,)
  S2(a)(i,k,m) += 1.0 sum(o2,o1,o3) D3(i,m,k,o2,o1,o3) * X(a)(o3,o2,o1,)
  Accumulate S2_(a)(i,k,m) for a
1 No 63
! S2(i,k,m,a) <--
! ( 1.00000000) D2(i,o1,k,o2) T2(o1,o2,o3,v1) V2(m,o3,a,v1)
! Indices of ERI are rotated to match with LHS.
! *** D2(i,o1,k,o2) T2(o1,o2,o3,v1) is skipped due to the priority Case 1 ..... X(i,o1,k,o2,m,o3,a,v1) <----- ( 1.00000000) D2(i,o1,k,o2) V2(a
,v1,m,o3)
! Polynomial order is O(o^6v^2)
! Maximum memory usage is O(o^6)
Case 2 ..... X(01,02,m,a) < ---- ( 1.00000000) T2(01,02,03,v1) V2(a,v1,m,o3)
! Polynomial order is O(o^4v^2)
! Maximum memory usage is O(o^3)
! The optimal choice is .....
1: X(o1,o2,m,a) <-- ( 1.00000000) T2(o1,o2,o3,v1) V2(a,v1,m,o3) 
2: S2(i,k,m,a) <-- ( 1.00000000) D2(i,o1,k,o2) X(o1,o2,m,a)
! Scaling
              : O(o^4v^2)
! Max size of X : o^3
! * Begin scaling analysis .... *
for a in {vir}:
 Read V2 from GA for a
  Read S2 from GA for a
  Declare X as a o^3 tensor
  for v1 in {vir}:
   Read T2 from GA for v1
   X_{(a)}(01,02,m) += 1.0 sum(03) V2(,v1,m,03) * T2(01,02,03,)
  S2_{(a)}(i,k,m) += 1.0 sum(o1,o2) D2(i,o1,k,o2) * X_{(a)}(o1,o2,m,)
  Accumulate S2_(a)(i,k,m) for a
! No.64
! S2(i,k,m,a) <--
! (1.00000000) D4(i,m,k,o3,o1,o4,o2,o5) T2(o4,o5,o1,v1) V2(o2,v1,o3,a)
! Indices of ERI are rotated to match with LHS.
! *** D4(i,m,k,o3,o1,o4,o2,o5) T2(o4,o5,o1,v1) is skipped due to the priority
Case 1 ..... X(i,m,k,o1,o4,o5,a,v1) < ---- (1.00000000) D4(i,m,k,o3,o1,o4,o5,a,v1)
o2,o5) V2(a,o3,o2,v1)
! Polynomial order is O(o^8v^2)
! Maximum memory usage is O(o^4)
Case 2 .... X(04,05,01,03,02,a) <---- ( 1.00000000) T2(04,05,01,v1) V2(a,
o3.o2.v1)
! Polynomial order is O(o^8v^1)
! Maximum memory usage is O(o^5)
```

```
eclipse sort.dat
 9 11, 12 16:46
                                                                  Page 141/145
Factorize: Conflict between choices of optimal memory usage and polynomial order
! The optimal choice is .....
1: X(o4,o5,o1,o3,o2,a) <-- ( 1.00000000) T2(o4,o5,o1,v1) V2(a,o3,o2,v1)
2: S2(i,k,m,a) <-- ( 1.00000000) D4(i,m,k,o3,o1,o4,o2,o5) X(o4,o5,o1,o3,o2,
! Scaling
             : O(o^8v^1)
! Max size of X : o^5
! * Begin scaling analysis .... *
for a in {vir}:
 Read V2 from GA for a
 Read S2 from GA for a
 Declare X as a o^5 tensor
 for v1 in {vir}:
   Read T2 from GA for v1
   X_{(a)}(04,05,01,03,02) += 1.0 sum() V2(,03,02,v1) * T2(04,05,01,)
 for i in {occ}
   for m in {occ}
     Read D4 from GA for i,m
     S2_{(a)}(i,k,m) += 1.0 sum(03,01,04,02,05) D4(,,k,03,01,04,02,05) * X_{(a)}(04)
,05,01,03,02,)
     Accumulate S2 (a)(i,k,m) for a
! No.65
! S2(i,k,m,a) <--
! ( 1.00000000) D3(i,o3,k,o2,o4,o1) T2(o3,o1,m,v1) V2(o2,a,o4,v1)
! Indices of ERI are rotated to match with LHS.
! *** D3(i,o3,k,o2,o4,o1) T2(o3,o1,m,v1) is skipped due to the priority
Case 1 ..... X(i,o3,k,o1,a,v1) <---- ( 1.00000000) D3(i,o3,k,o2,o4,o1) V2(
a.o2.o4.v1)
! Polynomial order is O(o^6v^2)
! Maximum memory usage is O(o^4)
Case 2 .... X(03.01,m.02.04,a) < ---- ( 1.00000000) T2(03.01,m.v1) V2(a.02)
,o4,v1)
! Polynomial order is O(o^7v^1)
! Maximum memory usage is O(o^5)
Factorize: Conflict between choices of optimal memory usage and polynomial order
! The optimal choice is .....
1: X(o3,o1,m,o2,o4,a) <-- ( 1.00000000) T2(o3,o1,m,v1) V2(a,o2,o4,v1)
2: S2(i,k,m,a) < -- (1.00000000) D3(i,o3,k,o2,o4,o1) X(o3,o1,m,o2,o4,a)
! Scaling
             : O(o^7v^1)
! Max size of X : o^5
! * Begin scaling analysis .... *
for a in {vir}:
 Read V2 from GA for a
 Read S2 from GA for a
 Declare X as a o^5 tensor
for v1 in {vir}:
   Read T2 from GA for v1
   X_{(a)}(03,01,m,02,04) += 1.0 sum() V2(,02,04,v1) * T2(03,01,m,)
 S2_{(a)}(i,k,m) += 1.0 \text{ sum}(03,02,04,01) D3(i,03,k,02,04,01) * X_{(a)}(03,01,m,02,01) 
4,)
```

```
eclipse sort.dat
 9 11, 12 16:46
                                                               Page 142/145
  Accumulate S2 (a)(i,k,m) for a
! No.66
! S2(i,k,m,a) <--
! ( 1.00000000) D3(i,o2,k,o3,o1,o4) T2(o4,o2,o1,v1) V2(m,v1,o3,a)
! Indices of ERI are rotated to match with LHS.
! *** D3(i,o2,k,o3,o1,o4) T2(o4,o2,o1,v1) is skipped due to the priority
Case 1 ..... X(i,o2,k,o1,o4,m,a,v1) < ---- ( 1.00000000) D3(i,o2,k,o3,o1,o4)
) V2(a,o3,m,v1)
! Polynomial order is O(o^7v^2)
! Maximum memory usage is O(o^6)
Case 2 ..... X(04,02,01,03,m,a) < ---- ( 1.00000000) T2(04,02,01,v1) V2(a,0)
3, m, v1)
! Polynomial order is O(o^7v^1)
! Maximum memory usage is O(o^5)
! The optimal choice is .....
1: X(04,02,01,03,m,a) < -- ( 1.00000000) T2(04,02,01,v1) V2(a,03,m,v1)
2: S2(i,k,m,a) < -- (1.00000000) D3(i,o2,k,o3,o1,o4) X(o4,o2,o1,o3,m,a)
             : O(o^7v^1)
! Max size of X : o^5
! * Begin scaling analysis .... *
for a in {vir}:
 Read V2 from GA for a
  Read S2 from GA for a
  Declare X as a o^5 tensor
  for v1 in {vir}:
   Read T2 from GA for v1
   X_{(a)}(04,02,01,03,m) += 1.0 sum() V2(,03,m,v1) * T2(04,02,01,)
 S2_{(a)}(i,k,m) += 1.0 \text{ sum}(02,03,01,04) D3(i,02,k,03,01,04) * X_{(a)}(04,02,01,03,01,04)
m,)
  Accumulate S2_(a)(i,k,m) for a
! No.67
! S2(i,k,m,a) <--
! (1.00000000) D3(i,m,k,o2,o1,o3) T2(o2,o3,o4,v1) V2(o1,v1,o4,a)
! Indices of ERI are rotated to match with LHS.
! *** D3(i,m,k,o2,o1,o3) T2(o2,o3,o4,v1) is skipped due to the priority
Case 1 .... X(i,m,k,o2,o3,o4,a,v1) < ---- ( 1.00000000) D3(i,m,k,o2,o1,o3)
V2(a,o4,o1,v1)
! Polynomial order is O(o^7v^2)
! Maximum memory usage is O(o^6)
Case 2 ..... X(02,03,01,a) < ---- (1.00000000) T2(02,03,04,v1) V2(a,04,01,a)
v21)
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^3)
! The optimal choice is .....
! Scaling
             : O(o^6v^1)
! Max size of X : o^3
! * Begin scaling analysis .... *
```

```
eclipse sort.dat
 9 11, 12 16:46
                                                              Page 143/145
for a in {vir}:
 Read V2 from GA for a
 Read S2 from GA for a
 Declare X as a o^3 tensor
 for v1 in {vir}:
   Read T2 from GA for v1
   X(a)(02,03,01) += 1.0 sum(04) V2(,04,01,v1) * T2(02,03,04,)
 S2_{(a)}(i,k,m) += 1.0 sum(02,01,03) D3(i,m,k,02,01,03) * X_{(a)}(02,03,01,)
 Accumulate S2 (a)(i,k,m) for a
! S2(i,k,m,a) <--
! ( 1.00000000) D2(i,o1,k,o2) T2(o2,o1,o3,v1) V2(m,v1,o3,a)
! Indices of ERI are rotated to match with LHS.
! *** D2(i,o1,k,o2) T2(o2,o1,o3,v1) is skipped due to the priority
Case 1 ..... X(i,o1,k,o2,o3,m,a,v1) <---- ( 1.00000000) D2(i,o1,k,o2) V2(a,o1,b)
,o3,m,v1)
! Polynomial order is O(o^6v^2)
! Maximum memory usage is O(o^6)
Case 2 ..... X(o2,o1,m,a) <---- ( 1.00000000) T2(o2,o1,o3,v1) V2(a,o3,m,v1
! Polynomial order is O(o^4v^2)
! Maximum memory usage is O(o^3)
! The optimal choice is .....
2: S2(i,k,m,a) < -- ( 1.00000000) D2(i,o1,k,o2) X(o2,o1,m,a)
! Scaling
            : O(o^4v^2)
! Max size of X : o^3
! * Begin scaling analysis .... *
for a in {vir}:
 Read V2 from GA for a
 Read S2 from GA for a
 Declare X as a o^3 tensor
 for v1 in {vir}:
   Read T2 from GA for v1
   X_{-}(a)(o2,o1,m) += 1.0 sum(o3) V2(,o3,m,v1) * T2(o2,o1,o3,)
 S2_{(a)}(i,k,m) += 1.0 \text{ sum}(01,02) D2(i,01,k,02) * X_{(a)}(02,01,m,)
 Accumulate S2_(a)(i,k,m) for a
! No.69
! S2(i,k,m,a) <--
     1.00000000) Ecas D3(i,m,k,o2,o1,o3) T2(o3,o2,o1,a)
! Indices of BareAmp are rotated to match with LHS.
1.a)
! Polynomial order is O(o^6v^1)
! Maximum memory usage is O(o^3)
! The optimal choice is ..... 
 1: S2(i,m,k,a) < -- ( 1.00000000)  Ecas D3(i,m,k,o2,o1,o3)  T2(o3,o2,o1,a) 
! Scaling
              : O(o^6v^1)
! Max size of X : o^3
```

```
eclipse sort.dat
 9 11, 12 16:46
                                                                 Page 144/145
! * Begin scaling analysis .... *
for a in {vir}:
 Read T2 from GA for a
 Read S2 from GA for a
 Declare S2 as a o^3 tensor
 S2_{(a)}(i, k, m) += Ecas sum(o2,o1,o3) D3(i,m,k,o2,o1,o3) * T2(o3,o2,o1,)
 Accumulate S2_(a)(i,k,m) for a
! No.70
! S2(i,k,m,a) <--
! ( 1.00000000) Ecas D2(i,o1,k,o2) T2(o1,o2,m,a)
! Indices of BareAmp are rotated to match with LHS.
Case 0 ..... S2(i,k,m,a) < ---- ( 1.00000000) D2(i,o1,k,o2) T2(o1,o2,m,a)
! Polynomial order is O(o^5v^1)
! Maximum memory usage is O(o^3)
! The optimal choice is \ldots\ldots
1: S2(i,k,m,a) < -- ( 1.00000000) Ecas D2(i,o1,k,o2) T2(o1,o2,m,a)
! Scaling
             : O(o^5v^1)
! Max size of X : o^3
! * Begin scaling analysis .... *
for a in {vir}:
 Read T2 from GA for a
 Read S2 from GA for a
 Declare S2 as a o^3 tensor
 S2(a)(i, k, m) += Ecas sum(o1,o2) D2(i,o1,k,o2) * T2(o1,o2,m,)
 Accumulate S2 (a)(i,k,m) for a
### SUMMARY ###
< Calculation of the overlap vector >
* 0 <oovv/oovv> 2 terms are generated ....
< Calculation of the diagonal elements starts >
* 0 L:oovv/R:oovv 31 terms are generated ....
* 1 L:ooov/R:ooov 45 terms are generated ....
< Calculation of the Sigma_{0} += <Psi0 | H T2 ER |Psi0> >
* 0 <g/oovv> 1 terms are generated ....
* 1 <g/oov> 5 terms are generated ....
< Calculation of the Sigma_{aa'}^{ee'} += <Psi0|EL H T0 |Psi0> >
* 0 <oovv/g> 1 terms are generated ....
* 1 <ooov/g> 5 terms are generated ....
< Construction of Sigma_{aa'}^{ee'} += <Psi0|EL H TR ER |Psi0> >
* 0 <oovv/oovv> 36 terms are generated ....
```

9 11, 12 16:46		eclipse_sort.dat	Page 145/145
* 1 <00vv/000v>	22 terms are		
* 2 <000v/00vv>	22 terms are	generated	
* 3 <000V/000V>	71 terms are	generated	
* Total number of	f terms : 243		