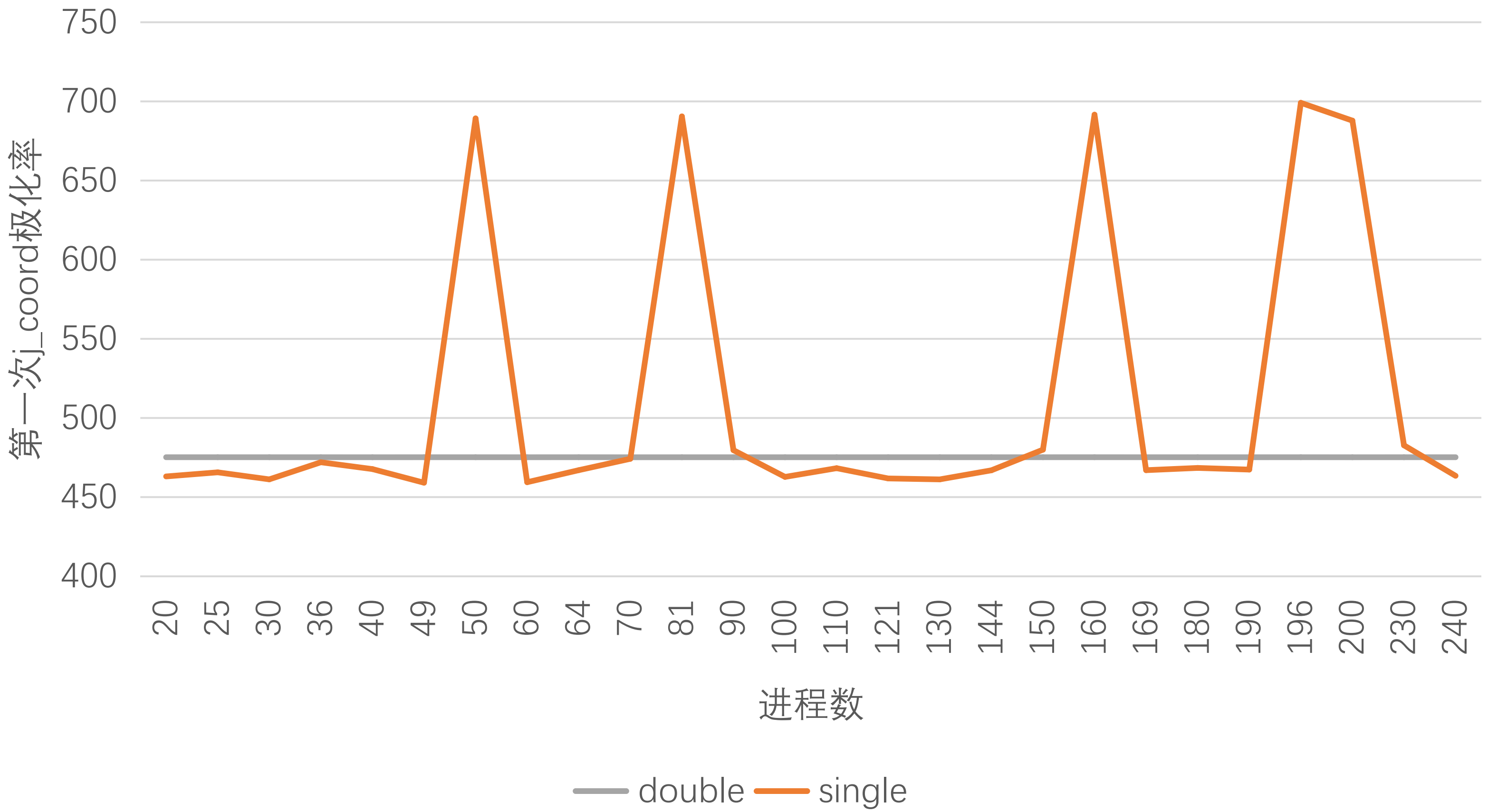
2021.9.27

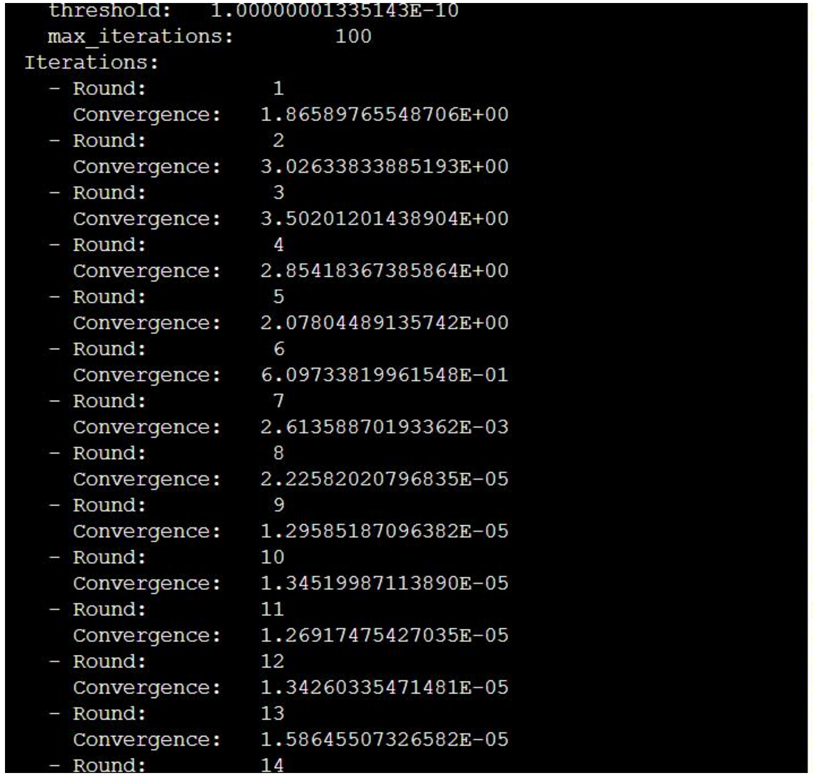
徐直前

单精度polar误差

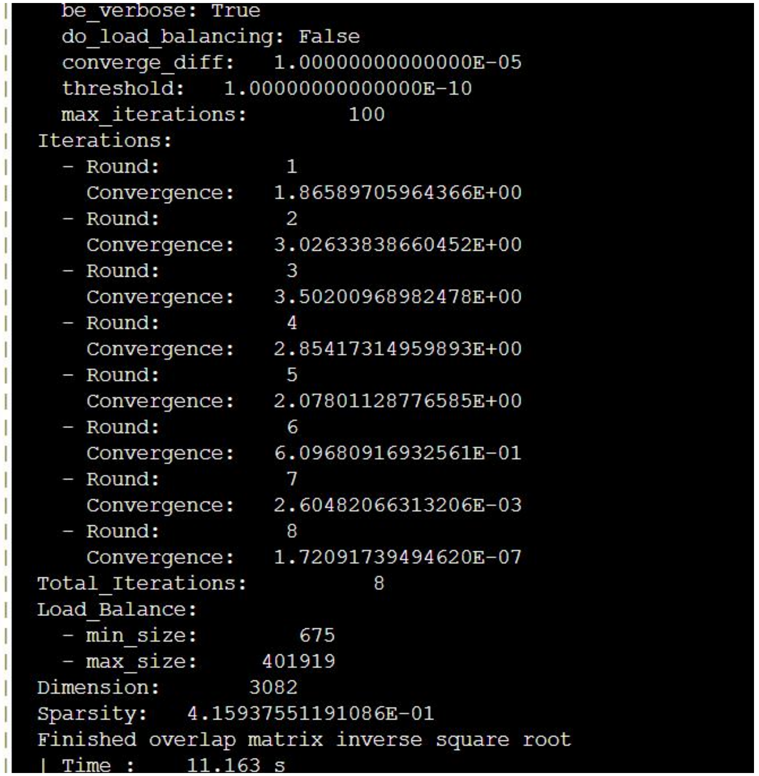


750
700
650
600
550
500
450
400
第一次j_coord极化率
20
25
30
36
40
49
50
60
64
70
81
90
100
110
121
130
144
150
160
169
180
190
196
200
230
240
进程数
double
single

单精度对Inverse square root的影响



```
  threshold:   1.00000001335143E-10
  max_iterations:        100
Iterations:
  - Round:          1
    Convergence:   1.86589765548706E+00
  - Round:          2
    Convergence:   3.02633833885193E+00
  - Round:          3
    Convergence:   3.50201201438904E+00
  - Round:          4
    Convergence:   2.85418367385864E+00
  - Round:          5
    Convergence:   2.07804489135742E+00
  - Round:          6
    Convergence:   6.09733819961548E-01
  - Round:          7
    Convergence:   2.61358870193362E-03
  - Round:          8
    Convergence:   2.22582020796835E-05
  - Round:          9
    Convergence:   1.29585187096382E-05
  - Round:         10
    Convergence:   1.34519987113890E-05
  - Round:         11
    Convergence:   1.26917475427035E-05
  - Round:         12
    Convergence:   1.34260335471481E-05
  - Round:         13
    Convergence:   1.58645507326582E-05
  - Round:         14
```



```
  be_verbose: True
  do_load_balancing: False
  converge_diff:   1.00000000000000E-05
  threshold:   1.00000000000000E-10
  max_iterations:        100
Iterations:
  - Round:          1
    Convergence:   1.86589705964366E+00
  - Round:          2
    Convergence:   3.02633838660452E+00
  - Round:          3
    Convergence:   3.50200968982478E+00
  - Round:          4
    Convergence:   2.85417314959893E+00
  - Round:          5
    Convergence:   2.07801128776585E+00
  - Round:          6
    Convergence:   6.09680916932561E-01
  - Round:          7
    Convergence:   2.60482066313206E-03
  - Round:          8
    Convergence:   1.72091739494620E-07
Total_Iterations:          8
Load_Balance:
  - min_size:        675
  - max_size:     401919
Dimension:       3082
Sparsity:   4.15937551191086E-01
Finished overlap matrix inverse square root
| Time :    11.163 s
```

神威上没有此现象，怀疑为Intel的MKL与神威上的Xmath有一定区别

Evaluate_first_order_C_polarizability的Scalapack版本

- 有两处，第一处在CPSCF_Loop之前，第二处在CPSCF_Loop中
- 将除了输入的矩阵之外的所有局部变量都改为Scalapack的分布式
- 最后将输出矩阵(first_order_density_matrix)通过pdlacp3整合为全局矩阵（即每个进程都有一份完整矩阵），也可通过aims里的sync_vector代替pdlacp3
- Ax=b中dgesv->pdgesv的过程中，由于dgesv的b向量是某全局矩阵tmp_B的每一列，为了避免多余通信，需要修改b向量的array descriptor，使得tmp_B的某一列正好在包含该列的进程中（本地数据），而不是scalapack默认的0号进程。解完后，再将b放回tmp_B从而得到解矩阵。
- n_basis = n_states <> n_occ_states？
- 在H2O体系下测试通过，误差在1e-10左右，大体系下还没测