409.6 million walkers

```
system read
electrons 54
spin-restrict 0
nonuniformrandexcits 4ind-weighted-part-exact
nobrillouintheorem
(hphf 1
molpromimic
endsys

calc
time 2715
methods
method vertex fcimc
endmethods
(nmcyc 100000)
diagshift 0.0
shiftdamp 0.1
 totalwalkers  4096e5
 STARTSINGLEPART 10000
(startcas 6,6
(walkcontgrow
 readpops
proje-changeref 1.2
 trial-wavefunction
(pops-trial  1000
   read-trial
 semi-stochastic
(  pops-core  100000
  read-core
tau 0.001 search
(max-tau 0.000005
truncinitiator
addtoinitiator 3
(shiftequilsteps 2000
maxwalkerbloom 1
allrealcoeff
realspawncutoff 0.3
memoryfacpart  2.5
memoryfacspawn  2.5
stepsshift 10
jump-shift
(definedet 1 2 3 4  6 14
en2-initiator
endcalc

integral
(partiallyfreezevirt  197,0
endint

logging
(write-core
(write-trial
binarypops
(compare-trial-and-fciqmc-amps
hist-excit-tofrom
(popsfiletimer 20
highlypopwrite 1000
printorboccs 1000
writeinitiators
calcrdmonfly 3 0000 1
(rdm-main-size-fac 0.01
(rdm-spawn-size-fac 0.01
(rdm-recv-size-fac 0.01
(hdf5-pops-write
(hdf5-pops-read
(write-spin-free-rdm
(diagflyonerdm
PRINTRODUMP
(printonerdm
endlog
end
```

```
 Procedure                    Calls       CPU    system     total
 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
 WalkerTime                    5640 137644.67      0.00 137644.67
 SyncTime                     11848   9774.53      0.00   9774.53
 AnnMainTime                   5640   6414.12      0.00   6414.12
 NECICUBE                         1   5323.56      0.00   5323.56
 POPS-write                       1   2307.38      0.00   2307.38
 CommsTime                     5640   1052.03      0.00   1052.03
 SortTime                      5640   1035.89      0.00   1035.89
 SemiStochCommsTime            5640    743.46      0.00    743.46
 Compress Sort interface       5640    691.79      0.00    691.79
 TrialInitTime                    1    349.62      0.00    349.62
 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
 Total                                165337.03      0.00 165337.03

 Global CPU time     165889.62
 Global system time       0.00
 Global total time   165889.62
 ================================================================
 Calculation ended 08/11/2018 at 20:53:58
 ================================================================
165889.62-349.62-2307.38-5323.56=157909.06 (walkerTime + SyncTime)
```

Switch to calcrdmonfly every 10 iterations:

```
 Procedure                    Calls       CPU    system     total
 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
 WalkerTime                    9720 131810.58      0.00 131810.58
 AnnMainTime                   9720   9357.87      0.00   9357.87
 SyncTime                     20008   7889.78      0.00   7889.78
 NECICUBE                         1   7468.16      0.00   7468.16
 POPS-write                       1   2278.44      0.00   2278.44
 CommsTime                     9720   1805.77      0.00   1805.77
 SortTime                      9720   1782.98      0.00   1782.98
 Compress Sort interface       9720   1191.80      0.00   1191.80
 SemiStochCommsTime            9720    924.92      0.00    924.92
 TrialInitTime                    1    349.22      0.00    349.22
 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
 Total                                164859.50      0.00 164859.50

 Global CPU time     165598.38
 Global system time       0.00
 Global total time   165598.38
 ================================================================
 Calculation ended 10/11/2018 at 18:56:53
 ================================================================
```

Switch to calcrdmonfly every 5 iterations:

```
 Procedure                    Calls       CPU    system     total
 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
 WalkerTime                    9020 133342.61      0.00 133342.61
 AnnMainTime                   9020   8991.71      0.00   8991.71
 NECICUBE                         1   7527.88      0.00   7527.88
 SyncTime                     18608   7075.01      0.00   7075.01
 POPS-write                       1   2339.47      0.00   2339.47
 CommsTime                     9020   1685.66      0.00   1685.66
 SortTime                      9020   1660.15      0.00   1660.15
 Compress Sort interface       9020   1106.01      0.00   1106.01
 SemiStochCommsTime            9020    954.58      0.00    954.58
 TrialInitTime                    1    349.27      0.00    349.27
 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
 Total                                165032.33      0.00 165032.33

 Global CPU time     165750.98
 Global system time       0.00
 Global total time   165750.98
 ================================================================
 Calculation ended 12/11/2018 at 17:05:47
 ================================================================
```

Without any RDM:

```
 Procedure                      Calls       CPU    system     total
 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
 WalkerTime                     12050 146130.98      0.00 146130.98
 SyncTime                       14389   7810.93      0.00   7810.93
 AnnMainTime                    12050   2841.18      0.00   2841.18
 POPS-write                         1   2303.67      0.00   2303.67
 SortTime                       12050   1959.73      0.00   1959.73
 Compress Sort interface        12050   1353.35      0.00   1353.35
 NECICUBE                           1   1229.64      0.00   1229.64
 CommsTime                      12050   1129.74      0.00   1129.74
 TrialInitTime                      1    344.17      0.00    344.17
 POPS-read                          1    212.91      0.00    212.91
 - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
 Total                                165316.30      0.00 165316.30

 Global CPU time     165537.52
 Global system time       0.00
 Global total time   165537.52
 ================================================================
 Calculation ended 04/11/2018 at 03:57:08
 ================================================================
```

```
N_iterations_without_RDM:   12050 in 165537.52 seconds = 13.74 seconds per iteration
N_iterations_RDM_every_10:   9720 in 165598.38 seconds = 17.04 seconds per iteraiton
N_iterations_RDM_every_5:    9020 in 165750.98 seconds = 18.38 seconds per iteraiton
N_iterations_RDM_every_1:    5640 in 165889.62 seconds = 29.41 seconds per iteraiton

Every_10: 9720*13.74 = 133553 seconds spent on non-RDM.  165598-133553 = 32045 seconds spent on RDM
Every_5:  9020*13.74 = 123935 seconds spent on non-RDM.  165750-123935 = 41815 seconds spent on RDM
Every_1:  5640*13.74 =  77494 seconds spent on non-RDM.  165889-77494  = 88105 seconds spent on RDM

Every_10:  32045/9720/10 = 0.33 seconds per RDM calculation
Every_5:   41815/9020/5  = 0.93 seconds per RDM calculation (why 3x  longer than 0.33 ?)
Every_1:   88395/5640/1  = 15.7 seconds per RDM calculation (why 45x longer than 0.33 ?)
```

Re-do above calculation but using WalkerTime instead of Global CPU time:

```
N_iterations_without_RDM:   12050 in 146130.98 seconds = 12.13 seconds per iteration
N_iterations_RDM_every_10:   9720 in 131810.58 seconds = 13.56 seconds per iteraiton
N_iterations_RDM_every_5:    9020 in 133342.61 seconds = 14.78 seconds per iteraiton
N_iterations_RDM_every_1:    5640 in 137644.67 seconds = 24.41 seconds per iteraiton

Every_10: 9720*12.13 = 117903 seconds spent on non-RDM.  131810-117903 = 13907 seconds spent on RDM
Every_5:  9020*12.13 = 109413 seconds spent on non-RDM.  133343-109413 = 23930 seconds spent on RDM
Every_1:  5640*12.13 =  68413 seconds spent on non-RDM.  137645-68413  = 69232 seconds spent on RDM

Every_10:  13907/9720/10 = 0.14 seconds per RDM calculation
Every_5:   41663/9020/5  = 0.53 seconds per RDM calculation (why 4x  longer than 0.14 ?)
Every_1:   69232/5640/1  = 12.3 seconds per RDM calculation (why 90x longer than 0.14 ?)

Furthermore, SyncTime is:
7810.93 for no-RDM,
7889.78 for every 10 steps,
7075.01 for every 5 steps,
9774.53 for every 1 step,

so there seems to be no correlation between SyncTime and how often we print RDM.
```