ストレージ構成による計算時間の比較

計算プログラム : ORCA 2.7.0 beta (OpenMPI)
OS : Fedora 10 (x86_64)

ストレージ構成	Overall	SCF iter.	MDCI module			
			FHT	SHT	SVC	MDCI total
A	18884.5 (100%)	171.9 (100%)	5888.5 (100%)	3485.9 (100%)	7513.7 (100%)	18771.6 (100%)
B	16134.0 (85.4%)	177.6 (103.3%)	4427.6 (75.2%)	2380.6 (68.3%)	7781.8 (103.6%)	15955.5 (85.0%)
C	14218.6 (75.3%)	181.3 (105.5%)	4046.9 (68.7%)	1975.9 (56.7%)	6822.7 (90.8%)	14036.2 (74.8%)
D	10420.8 (55.2%)	172.4 (100.3%)	1808.1 (30.7%)	1789.6 (51.3%)	5458.0 (72.6%)	10247.3 (54.6%)

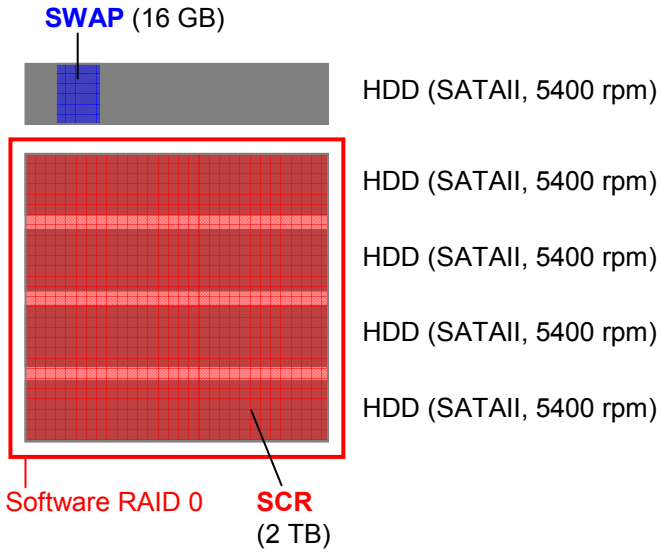
ワークステーションの主要構成パーツ

CPU : Intel Core2 Extreme QX9650 (3.00 GHz)
M/B : ASUS P5K PRO (P35)
RAM : CFD elixir W2U800CQ-2GL5J (PC2-6400 CL5 2 GB x 4)
VGA : Sapphire Radeon HD 3450
PSU : Seasonic SS-600HM

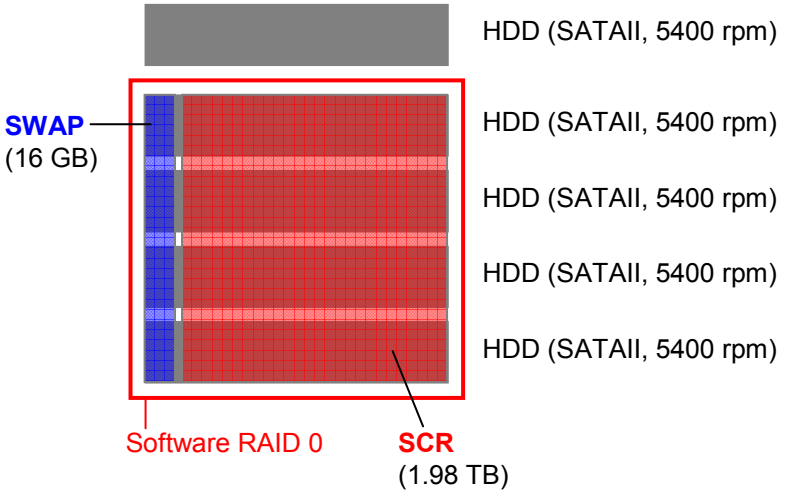
HDD : Western Digital WD5000AACS (SATAII, 500 GB, 5400 rpm)
SSD(1) : Intel X25-M SSDSA2MH080G2C1 (SATAII, 80 GB)
SSD(2) : SAMSUNG PB22-J MMCRE28G5MXP-0V (SATAII, 128 GB)

数値の単位は秒
FHT : First Half Transformation
SHT : Second Half Transformation
SVC : Sigma-vector Construction

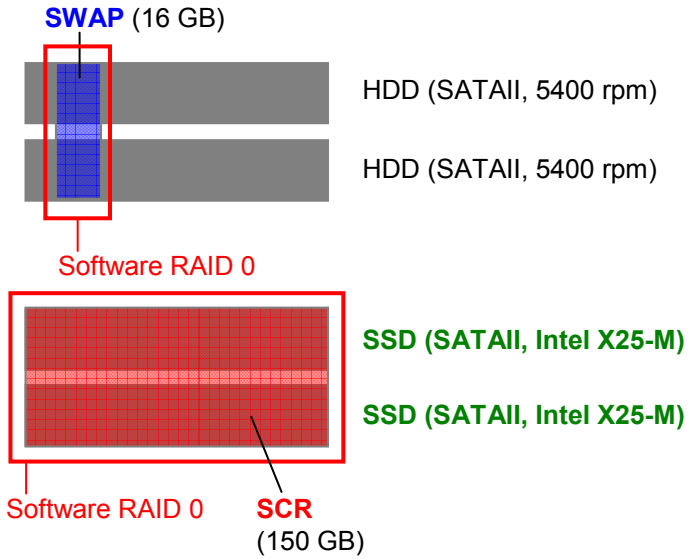
構成A



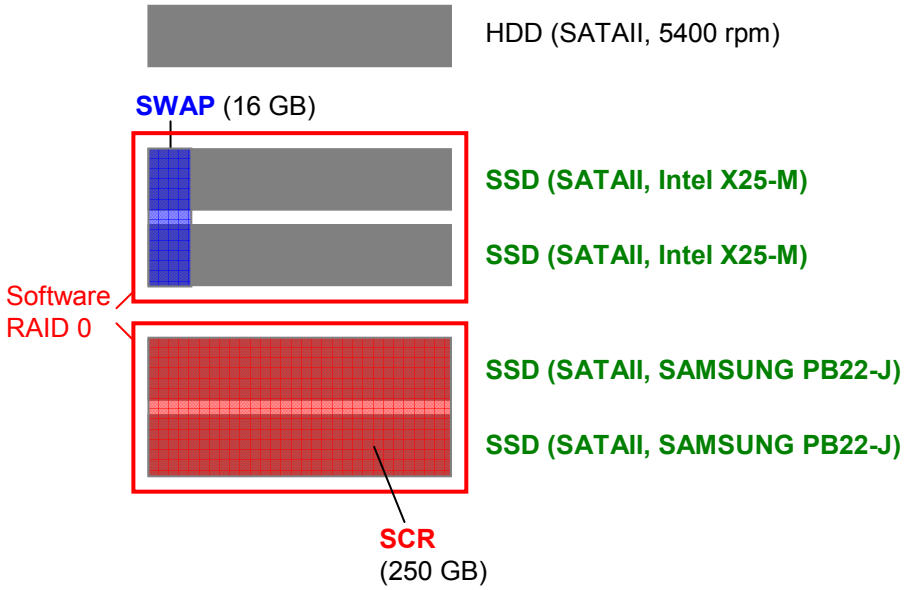
構成B



構成C



構成D



入力ファイル

```
! SP RHF RIJCOSX CEPA/1 aug-cc-pVDZ aug-cc-pVDZ/C
! TightSCF PAL4
%maxcore 1536
%mdci KCOpt KC_MO
    TrafoType trafo_full
    end
* xyz 0 1
O 2.196124 0.000000 -0.689324
C 1.390230 1.074380 -0.162300
C 1.390230 -1.074380 -0.162300
C 1.217950 0.674140 1.286220
C 1.217950 -0.674140 1.286220
H 1.835200 2.043400 -0.386450
H 1.835200 -2.043400 -0.386450
H 1.026800 1.350550 2.112840
H 1.026800 -1.350550 2.112840
C 0.035680 -0.764560 -0.901866
C 0.035680 0.764560 -0.901866
C -1.199320 1.153370 -0.128065
C -1.199320 -1.153370 -0.128065
O -1.861064 0.000000 0.312150
O -1.612610 2.257780 0.139220
O -1.612610 -2.257780 0.139220
H 0.031097 -1.221920 -1.895147
H 0.031097 1.221920 -1.895147
*
```

座標データは *J. Org. Chem.* **2005**, *70*, 6295.
のSupporting Informationより引用