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IBM DISTRIBUTION VERSION OF THE GAMESS AND MRD-CI CODES

by

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1. INTRODUCTION

The following notes describe the implementation and, in part, subsequent use of the SCF/GVB/MCSCF gradient code, GAMESS, and the multi-reference double excitation CI program, MRDCI. The present description is confined to the IBM version of theee programs, as currently running on the NAS AS/7000 at the Daresbury Laboratory.

The 9 track tape enclosed was written at 6250 bpi with IBM standard labels, vol=ser= . It contains 8 data sets, ae summarised in table 1, the IBM utility IEHMOVE having been used to unload each of the partitioned data sets to tape. An example job (as run on the AS/7000 under MVT) to move one of the files back to disk is shown in the Appendix.

The following notes provide an outline of the contents and role of each data set in implementing the packages. The aim is to ensure that the system can be installed and tested with no prior knowledge of the data requirements, or of the underlying quantum chemistry involved, with provision of a series of example joba and specimen output generated at Daresbury.

2. CONTENTS OF THE TAPE

a) The first data set on the tape, DSN = WAB.GAMESS.FORT, is an unloaded PDS containing the fortran and assembler source for the ALLDC and GAMESS programs (see table 2).

b) The second data set on tape, WAB.MRDCI.FORT, is an unloaded PDS containing the fortran and assembler source for the constituent programs of the MRD-CI package, namely TABLE, ADAPT, TRAN4, SELECT, CI, DIAG, NATORB, MOMENT, PROP1E, and the ATMOL programs MULL and PROP (see table 2) as operative with GAMESS AND MRDCI.

c) An unloaded PDS, DSN=WAB.GAMESS.LOAD, is the third data set on tape, comprising an NCAL load library which should be used as primary input to the link editor when creating the excutable modules of the ALLOC and GAMESS program. Note that this data set should be assigned to the link editor with DDNAME MFG. Note also that, with a single exception, all

fortran code has been compiled using the IBM extended-H compiler, with an optimization level OPT(2). The fortran source in member GETHES must, however, be compiled with OPT(1). With the exception of the source in ALLOCF, all code in the PDS WAB.GAMESS.FORT requires the compiler option AUTODBL to be set to DBL.

d) Ths fourth data set on tape, WAB.MRDCI.LOAD, is an unloaded PDS containing an NCAL library of the constituent programs of the MRD-CI package. Note the one to one correspondence between the member names of the NCAL library, and those of the fortran sources in WAB.MRDCI.FORT. Again all fortran code has been compiled using the extended-H compiler, with optimization level OPT(2): use of the AUTODBL feature in creating these programs is confined to the utility routines in members BASICF and BUFF2F.

In addition this NCAL load library contains primary input to the link editor for the ATMOL programs PROP and MULL (see table 2). In both cases the AUTODBL option DBL is required in regenerating the members.

e) The fifth data set on tape, WAB.LINKD.FORT, is an unloaded PDS containing the link edit instructions for each of the programs listed in table 2. Note that with the exception of the file allocator program, ALLOC, all programs require the link editor option OVLY. Again there is a one to one correspondence between the load module names and the member names of WAB.LINKD.FORT containing the link edit instructions. Inspection of these instructions for certain members of the MRD-CI package reveals a line of the form

INCLUDE SYSLIB(MANYDEVS)

This is required on the AS/7000 to allow use of fortran data sets with data set reference numbers in the range FT21 - FT50, and should clearly be removed if such use is permitted automatically at the user's installation.

3. IMPLEMENTING THE SYSTEM

The remaining data sets on tape are designed to assist in generating and testing the executable modules listed in table 2.

f) The sixth data set, DSN=WAB.LOADD.CNTL is an unloaded PDS containing

the JCL required to generate each of the executable modules, and to replace a given member of the appropriate NCAL load library (see members COMP, COMPASS and COMPAUTO).

Note that the PDS, WAB.DISTRIB.LOAD, has been assigned though the LIBRARY parameter of the FHCL procedure (as operative at Daresbury) to accept each executable load module: at other installations such a PDS should be assigned using DDNAME SYSLMOD. The JCL line

```
//C.SYSIN DD DUMMY
```

is specific to use of the FHCL procedure in a link-edit only fashion.

g) One possible problem which may prevent an executable module generated from the enclosed NCAL libraries running successfully at the user's installation originates from the differences between corresponding versions of the IBM I/O supervisor, so that the calling sequence to IBCOM generated at compilation time is incompatible with the version at the user's installation. This typically manifests itself with an OC1/OC4 abend at the outset of execution, when the programs commence data input. This situation may be remedied by recompiling the input data handling routines which instigate the links to IBCOM, and relinking the program with the revised NCAL member. Specifically, the following members will be involved in such a procedure,

(i) ALLOC - recompile WAB.GAMESS.FORT(ALLOCF)
(ii) GAMESS - recompile WAB.GAMESS.FORT(UTILIBMF)
(iii) MRDCI programs - recompile WAB.MRDCI.FORT(BASICF)

h) Access to the Date and Time-of-day routines available at the user's site may be made by inserting appropriate calls in the subroutine TIDAJO (member TIDAD of WAB.GAMESS.FORT and WAB.MRDCI.FORT), such that the R*8 arguments DATE and TIME are set to hollerith strings printable with AB format. At present these variables are set to blank strings.

4. EXECUTING THE PROGRAMS

(i) The seventh data set on the tape, DSN=WAB.EXAMPLES.FORT, is an unloaded PDS containing the JCL and data input for running a variety of test cases, as outlined in table 3. The corresponding line printer output produced by these jobs on the AS/7000 at Daresbury is included in the

eighth data set on tape, DSN=WAB.OUTPUT.FORT, where for convenience the output lines have been truncated to 80 character records.

Three of the jobs included in EXAMPLES must be executed prior to running the remaining examples:

(i) The member ALLOCATE contains the JCL for running the file allocator program, to be used in preallocating WAB.MFGMAIN and WAB.MFGDUMP, the mainfile and dumpfile used by GAMESS. The BLKSIZE of 13024 is appropriate to use on 3330 disk - a reasonable value for 3350 disks is 6160 (note the setting must be an integral number of R*8 words).

(ii) The member CREATE contains the JCL for creating the fortran data sets used by the MRD-CI programs, ADAPT, TRAN4, SELECT, CI, DIAG, NATORB, PROP1E and MOMENT.

(iii) The JCL and data input required to create the data set WAB.MRDCI.TABLE for use by the MRD-CI program CI is included in member DATABASE. This data set is output to FT01 by the program TABLE, and input in all subsequent runs of the program CI on FT43. It is only necessary to create this data set once on establishing the system. Note that this data set occupies approximately 200 tracks of 3330-1 disk space (1 track = 13030 Bytes).

Table 1. DATA SETS ON TAPE

Label	Space(*) Requirements	DSN	Purpose
1	774	WAB.GAMESS.FORT	Fortran and assembler source for GAMESS
2	262	WAB.MRDCI.FORT	Fortran and assembler source for MRDCI
3	370	WAB.GAMESS.LOAD	Load library for GAMESS
4	83	WAB.MRDCI.LOAD	Load library for MRDCI
5	5	WAB.LINKD.FORT	Link edit instructions for GAMESS and MRDCI
6	2	WAB.LOADD.CNTL	Specimen jobs for creating the executable load modules
7	11	WAB.EXAMPLES.CNTL	Specimen example jobs
8	302	WAB.OUTPUT.FORT	Line printer output from example jobs

(*) 3330-1 tracks (13030 Bytes)

Table 2. PROGRAMS COMPRISING THE GAMESS AND MRDCI SYSTEM

Name	Purpose
ALLOC	Disk allocator
GAMESS	SCF/GVB/MCSCF gradient program
TABLE	MRDCI TABLE Generator
ADAPT	MRD-CI Symmetry Adaption Program
TRAN4	MRD-CI Integral Transformation Program
SELECT	MRD-CI Configuration/Selection
CI	MRD-CI Hamiltonian Generator
DIAG	MRD-CI Diagonalisation/extrapolation program
NATORB	MRD-CI Natural Orbital program
MOMENT	MRD-CI Transition moment program
PROP1E	MRD-CI Properties program
MULL	Wavefunction analysis program
PROP	One-electron Properties program

APPENDIX. TRANSFER OF AN UNLOADED PDS TO DISK

```
//WABTAPE JOB (4510,WAB),GUEST,MSGCLASS=T,NOTIFY=WAB,
//  MSGLEVEL=1
// EXEC PGM=IEHMOVE,REGION=150K,TIME=(0,59)
//SYSPRINT DD SYSOUT=A,DCB=BLKSIZE=121
//FR DD VOL=SER=XXXXXX,UNIT=DEN6250,DISP=OLD,
//  DCB=(DEN=4,RECFM=FB,LRECL=80,BLKSIZE=800)
//TO DD UNIT=3330-1,VOL=SER=DL0210,DISP=OLD
//SYSUT1 DD VOL=SER=DL0210,UNIT=3330-1,DISP=OLD
//SYSIN DD *
 COPY PDS=WAB.MRDCI.FORT,FROM=DEN6250=(XXXXXX,2),TO=3330-1=DL0210,      C
               FROMDD=FR
/*
// EXEC NOTIFY,OPT=COND
//
```


Table 3. EXAMPLE JOBS AND OUTPUT IN WAB.EXAMPLES.CNTL AND WAB.OUTPUT.FORT

Member Name	Purpose
RUN1A	SCF calculation on the $X^1\Sigma^+g$ state of N_2, with subsequent symmetry adaption and integral transformation
RUN1E	4M/1R MRD-CI calculation on the $X^1\Sigma^+g$ state (T=30 uH)
RUN1C	Generation of natural orbitals and 1-electron properties
RUN2A	SCF supermatrix calculation of the $X^2\Sigma^+$ state of the OH radical in a (4s2p2d/2s2p) basis, with generation of a starting set of MOs from a closed shell calculation on OH^+.
RUN2B	Generation of an a.o. integral list, with subsequent symmetry adaption and integral transformation
RUN2C	Valence shell MRD-CI calculation of the $^2\Sigma^+$ state based on a 4M/1R (T = 20 uH) treatment
RUN3A	SCF supermatrix calculation of the X^1A_1 state of the NH_3 molecule in a (3s2p2d/2s1p) basis, subsequent generation of an a.o. integral list, with symmetry adaption and integral transformation
RUN3B	Valence shell MRD-CI calculation of the $1,2\,^1A_1$ states based on a 2M/2R (T = 30 uH) treatment
RUN3C	Generation of natural orbitals, properties and transition moment
RUN4A	SCF 4-31G calculation on the $^2A_1$ state of PH_4, preceded by a closed shell calculation on PH_4^+
RUN4B	CASSCF calculation on the $^2A_1$ state
RUN4C	Generation of symmetry adapted mainfile, integral transformation using the CASSCF MOs, and 1M/1R selection
RUN4D	Valence shell SDCI calculation
RUN4E	Generation of natural orbitals and 1-electron properties using PROP1E and PROP
RUN4F	Use of the Mulliken analysis program
RUN5	SCF and CASSCF geometry optimization of H_2O ($X\,^1A_1$) in a 3-21G basis set
RUN6	CASSCF calculation of the $2\,^3B_1$ state of CH_2 in a (4s2p/2s) basis. Initial orbitals generated from SCF calculations on the $^1A_1$ and $X\,^3B_1$ states