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PROGRAM CASCADE.

DESCRIPTION OF DATASETS FOR USE IN CRYSTAL DEFECT CALCULATIONS

by

M. LESLIE, Daresbury Laboratory

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Daresbury Laboratory

Daresbury, Warrington WA4 4AD

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1. INTRODUCTION

This document is a supplement to the previously published description of the input processor for the program CASCADE (Daresbury Laboratory technical memorandum DL/SCI/TM25T, Author: W. Smith). It describes in detail modifications and extensions made since this publication was produced. The major modifications are:

(i) More options for printed output have been added.

(ii) The program will now run PLUTO to relax the strains in the perfect crystal before running the defect calculation.

(iii) The amount of memory required for each job is easily changed. On the CRAY-1 this may be changed at run time without recompiling the program.

(iv) The energies of several defects may be calculated in the same job.

(v) It is possible to restart the job if the time limit or maximum number of iterations are exceeded.

2. OUTPUT OPTIONS

The output options have been modified and extended to give greater flexibility. The PRINT directive now has a format consisting of a number of keywords followed by an integer switch to indicate the level of printing required. In certain cases each digit of the integer is treated as a separate switch for a different part of the program. The IDUMP value is added to the integer (or digit) to increase the amount of output for all of the keywords. A list of the keywords with the possible switch values and the default is given below.

LATT
- 0 No output
- >0 The symmetry matrices of the point group of the lattice vectors are printed.

Default 0.

BASI
- 0 The basis species, defects and origin are output by default.
- >0 The list of basis species is output after sorting into species types and after the shift of origin. The point group matrices of the basis atoms about the specified origin are listed.

The point group matrices of the defect about the origin are listed.

Default 0

REG1 REG2 These switches are both three digit integers where the unit digit refers to the crystal definition phase, the tens digit to the iterative phase and the hundreds digit to the final cycle of the iterative phase. The values of the switches are as follows

0 No output

1 The first ten symmetry classes of each species type are listed.

2 All classes are listed.

3 All members of all classes are listed.

Defaults REG1 202

REG2 101

RECI

0 No output

1 List the first ten reciprocal lattice vectors.

2 List all reciprocal lattice vectors

3 List all symmetry related reciprocal lattice vectors.

Default 2

SYMM

0 No output

1 List symmetry information

Default 0

CLAS

0 No output

1 Output various lists of classes of atoms.

Default 0

PLUT This switch is a five digit integer.

Numbering the digits from right (units digit) to left the digits have the following values and meanings.

Digit 1 0 No output

1 List the basis and bulk strains before the first iteration and after the last iteration of PLUTO

2 List the basis and bulk strains each cycle.

Digit 2 As for digit 1 but listing the elastic constant tensor and dielectric constant tensors.

Digit 3 0 No output

1 List the tensors used in the calculation of region 2 displacements after the last cycle.

Digit 4 0 No output

1 List the force constant matrix before the first cycle and after the last cycle.

2 List the force constant matrix on every cycle of PLUTO.

Digit 5 0 No output

1 List, for each basis atom, the Madelung energy, the short range energy and the contribution to the energy of region 2.

The lattice energy is always listed by default.

Default value 00012

STRU

0 No output

1 Output the structure factors

Default 1

MATR A three digit integer which controls output of the second derivative matrix and its inverse from the defect energy calculation. The units digit refers to the second derivative matrix before inversion, the tens digit to the inverse and the hundreds digit to the updated inverse. The digits may take three values.

0 No output

1 List the gradient vector only

2 List the second derivative matrix or its inverse.

Default 0

ENGY

0 Output only the total defect energy each cycle.

1 Output the various contributions to the defect energy each cycle. Also the interstitial coordinates will be listed each cycle.

Default 0

3. PLUTO ITERATION

An option has been added to CASCADE to allow the user to relax the strains in the lattice before entering the defect energy calculation. Either the positions of the basis atoms in the unit cell or the lattice vectors or both of these may be relaxed to eliminate basis or bulk strains respectively. The iteration is controlled using the START PLUT directive which now has the format

START PLUT int bsinc bkinc litt1 litt2

int is an integer giving the number of times the PLUTO calculation is carried out. (int = 1 therefore does not carry out any iteration). This is the default.

bsinc, bkinc

These are two real numbers giving the factors by which the calcualted displacements are muitiplied before updating the position vectors of the basis atoms or the lattice vectors respectively. Values of 0.0 in either field will keep the appropriate vectors fixed.

litt1

is a four character literal which can have the following values.

NONE	No species will be relaxed.
ALL	All species will be relaxed.
CORE	Relax the cores and shells treating the ion as one unit so that no additionai core-shell displacements are set up.
SHEL	Relax the shells only keeping the cores fixed.
litt2	is a four character literal which identifies the substance if potentials for more than one substance have been read in. iitt2 may be omitted if only one substance is being considered.

If the PLUTO iteration option is selected then the order of the directives in the CASCADE dataset is slightly different to that normally used. The order must now be

LATTICE VECTORS BASIS VECTORS DEFECTS | POTENTIAL INFORMATION | PLUTO | CRYSTAL DEFINITION | RELAXATION

The order normally used is

LATTICE VECTORS BASIS VECTORS DEFECTS | CRYSTAL DEFINITION | POTENTIAL INFORMATION | PLUTO | RELAXATION

If a PLUTO iteration is not carried out either card order is acceptable. It is possible to stop the calculation after the PLUTO phase simply by inserting a STOP directive in the dataset.

Finally, for implementation on the CRAY-1 only, if PLUTO does carry out iterations, the program will attempt to write to FORTRAN unit 8 a list of the updated lattice vectors and basis vectors in a format suitable for inclusion in a CASCADE dataset. Therefore if int is greater than 1, the user must ensure that the CRAY JCL ASSIGN UNIT 8 is used, even if the updated vectors are not required.

This is because the WRITE(8,....) statement will open unit 8 for output and reserve space for the I/O buffers which lies in the space used by the blank common block, and the job will ABORT at a later stage. (See below).

4. ALLOCATION OF MEMORY

Although CASCADE has been written in such a way that it will be possible to implement dynamic core allocation at run time, this has not yet been done. For operation on machines other than the CRAY-1, the integer read in on the DIMENSION card should be the same as the size of the array ISPACE, which is defined in the main segment of the program.

For operation on the CRAY-1, a DIMENSION card is still needed, although the integer value read in has no effect on the running of the program. The user nevertheless does have some control over the size of the program. This is done by requesting a field length for the program using the RFL,M=fl. card in the CRAY JCL. (See CRAY-OS Reference Manual SR-0011 Part 2 2-4.) fl is an octal integer giving the number of blocks (1000_8 words) into which the program is loaded. The maximum value is 1370. The size of

the blank common block is then determined by reading the relevant constants in the job communication block (see CRAY FORTRAN Reference Manual 2240009 page 3-68.7 and CRAY-OS Reference Manual SR-0011 Apendix A). This array is then used as storage for all the large arrays used by the crystal definition, PLUTO and relaxation sections of the program.

The only difficulty which can arise is that, if a file is opened after the size of the common block has been determined, then space is reserved for the I/O buffers in the upper part of the user field. This may cause the logical file tables (LFT's) to be overwritten and the job to abort. This problem can be avoided by including an ASSIGN card in the CRAY JCL for any FORTRAN unit number to which data may be written or from which data is read. Units 5 and 6 are automatically assigned. The other unit numbers and the circumstances under which they are used are given in Table 1.

TABLE 1

Unit Number	Nature of I/O	Use
7	WRITE (FORMATTED)	Provide a graphics dataset if a PLOT directive is in the CASCADE dataset.
8	WRITE (FORMATTED)	Produce an updated set of lattice and basis vectors from PLUTO. (See part 3 of this manual).
9	WRITE (UNFORMATTED)	Write a relaxed coordinate dump if a WRDU directive is in the CASCADE dataset.
10	READ (UNFORMATTED)	Restart a job from a coordinate dump. (See part 9 of this manual).

If the field length specified is too small, the program will terminate, but it will attempt first to determine the field length needed for the job step in which the run terminated. A successful run will also print the minimum field length needed for the job. This value can then be used if the same or a similar job is run.

5. REGION ONE SIZE SPECIFICATION

The format of the REGI card has been slightly altered. There are now 8 operands instead of 7. The first parameter was the number of classes of atoms required in region 1. This is replaced by two new operands. The first is a four letter keyword and the second is an integer or real variable depending on the keyword. The keywords and variable types needed are

Keyword	Variable Type	Meaning
CLAS	Integer	Number of classes in region 1.
ATOM	Integer	Number of atoms in region 1
RADI	Real	Radius of region 1

If the keyword is omitted the program assumes the CLAS option is being used.

6. RECORD LENGTH SPECIFICATION

Datasets containing standard IBM line numbers (in columns 73-80) may be used. The input processor reads 80 characters per card image, which may lead to problems if the line number is interpreted as data. To avoid this problem a new directive IREC has been implemented. The format is

IREC int

where int is an integer (<80) which specifies the number of characters read in from each record. For a line numbered dataset the directive

IREC 72

should be included either before or after the title.

7. OPTIONS FOR CALCULATING MORE THAN ONE DEFECT ENERGY IN THE SAME JOB

Several options are available to allow the calculation to continue after the first START RELA card. These are

(a) Calculate the defect energy with a new region size.

(b) Calculate the defect energy with a new potential cut-off.

(c) Calculate the energy of the same defect in a different crystal.

(d) Calculate the energy of a different defect in the same crystal.

7(a) NEW REGION SIZE SPECIFICATION

The energy of the defect may be recalculated using a larger region size. The relaxed crystal coordinates may be used as a starting point for the new calculation. In order to re-use the relaxed coordinates a RESTART directive is placed immediately after the START RELA directive. New region sizes must be read in using a REGN diretive which has the format
REGN litt param1 param2.

Litt and param1 specify the new region 1 size as described in Section 5 of this manual. (Litt may be omitted, in which case the CLAS option is assumed). Param2 is the new region 2 radius. Both region sizes must either stay the same or increase. The dataset should then contain a START CRYS and START RELA directive. A typical dataset would be

```
  .
  .
  .
REGI  RADI 1.2 2.4 .....
START CRYS
  .
  .
START RELA
RESTART
REGN  RADI 1.3 2.6
START CRYS
START RELA
  .
  .
```

Convergence in the new region size is usually very rapid, which can result in a considerable saving in CPU time.

7(b) NEW POTENTIAL CUT-OFF

To calculate the defect energy with a new potential cut-off a CUTO directive is used. This has the format CUTO param1 param2 param3 param4

where parameters 1-4 have the following meanings

parameter1	New short range potential cut-off
parameter2	New maximum permissible core-shell separation.
parameter3	New maximum permissible core displacement.
parameter4	New maximum range of potentials.

This is followed by a START PLUT and START RELA directive. The short range potential cut-off should not equal an atom-atom separation in the crystal.

7(c) MORE THAN ONE SUBSTANCE

It is possible to calculate in one job the energies of defects in two or more crystals with the same structure. All the potentials are read in with one call to POTE. It is necessary to specify the lattice constant appropriate to a set of potentials. This is done using a new sub-direction LCON which has the format
LCON litt rlat
where litt is a literal which is used to identify the substance (only the first four characters will be read) and rlat is the lattice constant. The sub-directive LCON must be placed after the species have been read in but before any potentials are read in. The value of LCON read in here overrides that read in on the REGI card. The literal litt must also be supplied on the START PLUT card (see section 3). A maximum of ten lattice constants may be given per run. If the potentials for only one substance are read in, the LCON sub-directive may be omitted. If two substances share a common ion, the potential must be read in twice with a different species label. This is beause the potentials are scaled by the lattice constant to carry out the perfect lattice and defect calculations.

In order to continue the calculation with a new substance it is necessary to re-label the basis species. This is done using the RELB sub-directive in POTE. The RELB card is followed by cards needed to re-label all of the basis atoms. These cards have the format
Oldlabel Newlabel Species (Defect)
where oldlabel is the old species label, e.g. NA+
Newlabel is the new species label e.g. K+
Species is CORE or SHEL

(Defect) is an optional additional parameter (see 7(d) below).

The re-labelling is terminated by an ENDS sub-directive and the potential input routine is then terminated by an additional ENDS card. The directives required after this card are as follows

```
DEFECT
  .
  .
New defect                Optional - Needed if a new defect is defined.
information
  .
  .
ENDS

CUTO                      Optional - needed if the potential cut-off is
                          different.
START  PLUT ..............................  litt.
                          Necessary - litt must agree with the literal
                          given on the LCON directive.
REGN                      Optional - Needed if the crystal regions are
                          changed.
START CRYS                Only needed if there is a new DEFECT or REGN
                          directive.
START RELA
```

An example of a dataset is given below.

```
DIME   180000
CUBI
REGI   RADI   3.0   6.0   2.722   1.5   0.1   1.5   2.0
THERMAL
LATT
1.0    1.0    0.0
1.0    0.0    1.0
0.0    1.0    1.0
BASI
CA2+   CORE   0.0   0.0   0.0
F-     CORE   0.5   0.5   0.5
F-     CORE   0.5   0.5  -0.5
CA2+   SHEL   0.0   0.0   0.0
F-     SHEL   0.5   0.5   0.5
F-     SHEL   0.5   0.5  -0.5
CENTRE        0.5   0.5   0.5
ENDS
DEFECT
F-     CORE   VACA  0.5   0.5   0.5
F-     SHEL   VACA  0.5   0.5   0.5
ENDS
START  CRYS
POTE
SPEC
SR2+   CORE   -3.0378   1.0
CL-    CORE    1.519    1.0
SR2+   SHEL    5.0378   0.0
CL-    SHEL   -2.519    0.0
CA2+   CORE   -3.24     1.0
F-     CORE    1.38     1.0
CA2+   SHEL    5.24     0.0
F-     SHEL   -2.38     0.0
ENOS
LCON   SRCL2   3.588
BUCK   SR2+   SHEL    CL-   SHEL
2250.3      0.3397      0.0      6.0
ENDS
BUCK   CL-    SHEL    CL-   SHEL
1227.18     0.3214      0.0      6.0
ENDS
HARM   SR2+   CORE   SR2+   SHEL   111.9
HARM   CL-    CORE   CL-    SHEL    35.99
LCON   CAF2     2.722
BUCK   CA2+   SHEL   F-     SHEL
1329.6      0.2979      0.0      5.0
ENDS
BUCK   F-     SHEL   F-     SHEL
1808.0      0.293             109.1
```

```
ENDS
HARM   CA2+   CORE   CA2+   SHEL   390.9
HARM   F-     CORE   F-     SHEL   101.2
ENDS
START  PLUT   1      0.0    0.0    NONE   CAF2
START  RELA
POTE
RELB
CA2+   SR2+   CORE
F-     CL-    CORE
CA2+   SR2+   SHEL
F-     CL-    SHEL
ENDS
ENDS
START  PLUT   1      0.0    0.0    NONE   SRCL2
START  RELA
STOP
```

7(d) MORE THAN ONE DEFECT

Two options are available for carrying out such calculations.

Option (i)

This option may be used if it is not necessary to repeat the START CRYS directive. The new defect must have exatly the same unrelaxed co-ordinates as the old defect and the crystal regions for the relaxation will be the same. This option could be used if the energies of several foreign interstitials wre needed. The RELB sub-diretive of POTE is used (see section 7(c)). The RELB card is followed by any number of cards with format

Oldlabel Newlabel Species Defect

The first three parameters have the meanings given in 7(c). Defect is INTE or INTF to indicate that the species is an interstitial. An interstitial which is also an atom of the host lattice can be re-labelled a foreign interstitial in this way without re-labelling the basis atoms. An example of a re-labelling sequence is given below

.
.
.


```
START  RELA
POTE
RELB
FE3+   TI3+   CORE   INTE
FE3+   TI3+   SHEL   INTE
ENDS
ENDS
START  RELA
POTE
RELB
TI3+   MG2+   CORE   INTE
TI3+   MG2+   CORE   INTE
ENDS
ENDS
START  RELA
STOP
```

Option (ii)

In cases other than that described above the user will need a new DEFECT directive and coordinates, a new START CRYS directive and a START RELA directive. The new defect must have the same origin and the same or lower symmetry.

B. COORDINATE DUMP AND RESTART

CASCADE will dump the relaxed coordinates so that a restart may be made under the following circumstances.

i) The jobtime would be exceeded on the next iteration cycle.
ii) The maximum number of iterations is exceeded.
iii) The core shell separation has exceeded the limit set by the REGI directive.
iv) The core displacement for one ion has exceeded the limit set by REGI.

The CRAY JCL necessary to carry out the dump and restart is described in section 10. A dump is written using an unformatted write to FORTRAN unit 9. To obtain a dump a WRDU directive must be included anywhere in

the dataset before the START RELA directive. This will produce a dump even if the job terminates successfully. The dump is read to FORTRAN unit 10. To read a dump file a REDU directive must be placed in the dataset immediately after the DIMENSION directive. The restart dataset must otherwise be exactly the same as that which produced the dump, except that the region sizes may be increased as described in section 7(a).

9. SUMMARY OF CARD ORDER

DIRECTIVE	PREREQUISITE CALL
IREC	
TITL	
DUMP	
PRIN	
MAXI	None - Optional directives
PLOT	
ACCU	
REDU	
WRDU	
DIME	
CUBI or HEXA	
REGI	None - Mandatory directives
OPTI or THER	
LATT	HEXA or CUBI
BASI	LATT, REGI, DIME
DEFE	BASI
POTE	DEFE
PLUT	POTE, THER or OPTI
CRYS	DEFE, PLUT if int > 1
RELA	CRYS, PLUT

After the first call of RELA, the following sequences are possible.

DIRECTIVE	MANDATORY FURTHER DIRECTIVES
RESTART	REGN, CRYS
REGN	CRYS
DEFECT	CRYS
CUTO	PLUTO
POTE-RELB (Interstitials)	None
POTE-RELB (Basis)	PLUTO

10. EXAMPLES OF CRAY JCL

The load module is stored as a permanent dataset on the CRAY disc with a PDN CASCBN under userid LL. The minimum JCL required is given below.

Example 1

```
JOB, JN=useridJOB, US='acct,userid',T=60.
RFL,  M=300.
ACCESS, DN=BIN, PDN=CASCBN, ID=LL.
BIN.
/EOF
                        data
/EOF
/EOJ
```

The RFL control statement is discussed in section 4 of this manual.

The second example gives the JCL needed to write a new set of basis coordinates after the PLUTO iteration has been carried out. The JCL for the PLOT option is similar, although the unit number is FTO7.

Example 2

```
JOB, JN=useridJOB, US='acct,userid', T=60.
ASSIGN, DN=F1, A=FT08.
RFL, M=400.
ACCESS, DN=BIN, PDN=CASCBN, ID=LL.
BIN.
DISPOSE,DN=F1,DC=ST,DF=CB,ID=userid,WAIT, †
```

```
TEXT= 'DSN=userid.PLUOUT.DATA,DISP=(NEW,CATLG)', +
'UNIT=3330-1,VOL=SER=DL0295,SPACE=(TRK(1,1))', +
'DCB=(RECFM=FB,LRECL=80,BLKSIZE=3120)'.
/EOF
                                    data
/EOF
/EOJ
```

The following two examples give the JCL needed to dump the coordinates and to restart after a dump

Example 3: Coordinate dump

```
 10    JOB,JN=useridJOB, US='acct,userid', T=60.
 20    ACCESS,DN=DELETE,PDN=CDUMP,ID=userid,UQ.
 30    DELETE,DN=DELETE.
 40    END.
 50    EXIT.
 60    ASSIGN, DN=C1,A=FT09.
 70    RFL, M=400.
 80    ACCESS,DN=BIN,PDN=CASCBN,ID=LL.
 90    BIN.
100    REWIND,DN=C1.
110    SAVE,DN=C1,PDN=CDUMP,ID=userid.
120    /EOF
```

Lines 20-50 delete an existing permanent dataset called CDUMP (See Daresbury Computer Users Guide, Chapter 10, 10.7 Example B, Page 41).

Example 4: Restart

```
JOB,JN=useridJOB, US='acct,userid', T=60.
ACCESS,DN=C1,PDN=CDUMP,ID=userid.
ASSIGN,DN=C1,A=FT10.
ACCESS,DN=BIN,PDN=CASCBN,ID=LL.
RFL, M=400.
BIN.
/EOF
```


11. CONVERSION OF HADES DATASETS TO THE CASCADE FORMAT

Introduction

A FORTRAN program has been written to run on the NAS at Daresbury to convert existing datasets to the format needed to run CASCADE. The existing HADES dataset formats are summarised in Appendix A. They will be referred to as HADES III (UCL), HADES II and HADES III (ICI). Before going into detail some general information about the conversion is given below.

(i) Defect Origin

The defect coordinates for a CASCADE dataset are given with respect to the same origin as the basis atoms. For a HADES III dataset the defect coordinates are given with respect to the origin which is read in. The conversion program carries out the necessary subtractions. For a HADES II dataset no origin is read in. The function of the origin is to define the symmetry since the point group is determined by CASCADE and HADES about this point.

(ii) Region Sizes

For HADES III (UCL) up to 5 region 1 sizes may be read in. The conversion program takes the last (largest) of these values for the CASCADE dataset. The region 1 size is defined as the number of species (i.e. cores and shells) in region 1, and the CASCADE dataset is written using the number of atoms option with this value. The region 2 radius is read in twice in the HADES dataset. If there is only one region 1 size given the second value of the region 2 radius is ignored, otherwise it is this value which is used.

For HADES II it is again possible to have more than one region 1 size and again the conversion program takes the last (largest) value. The region 1 size is defined as the number of classes of ions in region 1. This value is doubled to give the number of cores and shells and written to the CASCADE dataset using the number of classes option.

For HADES II (ICI) the region 1 size is read in once only as a radius and written to the CASCADE dataset with the radius option.

(iii) Potential Information

Any species type, potential type or spring constant which is found not to correspond to a basis or interstitial species is ignored.

(iv) Fixed Interstitials

For HADES II datasets only, any interstitial with a negative type number will be marked as a fixed interstitial in the CASCADE dataset.

(v) Specification of more than one Potential

Again only for HADES II, more than one list of potential information may be specified. Any one of these lists may be selected for output.

(vi) Limits on the Array Sizes in the Conversion Program

The maximum number of data cards which may be processed are as follows

BASIS ATOMS	200
VACANCIES	10
INTERSTITIALS	10
SPECIES TYPES	20
POTENTIAL TYPES	20
HARMONIC INTERACTION TYPES	20

(vii) A CRAY END-OF-FILE card (/EOF) and END-OF-JOB card (/EOJ) are written at the end of the CASCADE dataset.

Details of Running the Program

(i) CLIST and JCL needed to run the program

The program is designed to run either interactively or in batch mode. In the interactive mode the program will type questions on the user teletype to which the user responds. In batch mode the responses must be input into a separate dataset which the program can access at run time. The load module is stored in 'LL.LOAD(CONV)'.

(ii) Interactive Mode

A CLIST which will run the program is given below

```
PROC 2 DS1 DS2
FA
FREE F(FT05F001 FT06F001 FT07F001) ATTRLIST(ATTR)
ATTRIB ATTR BLKSIZE(3120) LRECL(80) RECFM(F,B)
ALLOC FILE(FT05F001) DA(&DS1..DATA) SHR
ALLOC FILE(FT06F001) DA(*)
ALLOC FILE(FT07F001) DA(&DS2..DATA) NEW TRACKS-
```



```
 SPACE(1,1) USING(ATTR)
ALLOC FILE(FT08F001) DA(*)
ALLOC FILE(FT09F001) DA(*)
CALL 'LL.LOAD(CONV)'
END
```

If this CLIST is input into a file userid.CLIST(CONVERT) and the user has an existing dataset OLDFILE.DATA then this may be converted to NEWFILE.DATA by typing CONVERT OLDFILE NEWFILE.

USER RESPONSES

After a short while during which the files are allocated the program will begin to type questions on the user terminal. The questions and responses are given below; responses by the user are underlined.

```
TYPE DATASET FORMAT TYPE, I1
1= UCL HADES3, 2 = UCL HADES2, 3 = ICI, 4 = UCL HADES3 NEW
1
FORAMT FOR SPECIES LABEL IS 2A4
CHARACTERS 1-4 ARE ION TYPE
EG NA+, CL-, SR2+. THE LABEL MUST NOT CONTAIN ANY SPACES
CHARACTERS 5-8 ARE CORE OR SHEL
TYPE SPECIES LABEL FOR TYPE NO    1
NA+ CORE
TYPE SPECIES LABEL FOR TYPE NO    2
NA+ SHEL
TYPE SPECIES LABEL FOR TYPE NO    3
CL- CORE
TYPE SPECIES LABEL FOR TYPE NO    4
CL- SHEL
TYPE MAXIMUM CORE DISPLACEMENT ALLOWED DURING REFINEMENT, F12.6
2.0
TYPE NUMBER OF TIMES PLUTO CALCULATION IS CARRIED OUT
INCREMENTS ON THE BASIS AND BULK STRAINS PER CYCLE
INCREMENT SWITCH (CORE,SHEL,ALL,NONE)
FORMAT(I4,2F8.4,1X,A4)
   1     0.0     0.0 NONE
TYPE OUTPUT SWITCHES IF DEFAULTS ARE NOT WANTED, OPTIONS ARE
```

```
REG1,REG2,RECI,SYMM,PLOT,CLAS,LATT,BASI,STRU,MATR
FORMAT IS A4,1X,I5, WHERE THE I5 FIELD CONTAINS THE SWITCH VALUE
TERMINATE WITH END
IF NO SWITCHES ARE WANTED JUST TYPE END
ALSO TYPE PLOT IF A PLOT DATASET IS WANTED FROM THE CASCADE RUN
REG1   212
REG2   212
PLOT
END
```

For HADES II datasets the questions and responses are slightly different. After typing the dataset type (2), the questions are

```
THERE ARE     2 LISTS OF POTENTIAL DATA
TYPE WHICH LIST IS REQUIRED, I1
1
FORMAT FOR SPECIES LABEL IS A4
EC NA+, CL-, SR2+. THE LABEL MUST NOT CONTAIN ANY SPACES
TYPE SPECIES LABEL FOR TYPE NO    1
CA2+
TYPE SPECIES LABEL FOR TYPE NO    2
F-
TYPE MAXIMUM ALLOWED CORE-SHELL SEPARATION, F12.6
0.1
```

The questions and responses are then the same starting from TYPE MAXIMUM CORE DISPLACEMENT ALLOWED .....

BATCH MODE

A CNTL file for running the job in batch mode is given below. The user responses given above for the interactive mode are assumed to have been input into the file userid.CONFILE.DATA

```
//useridJOB JOB (acct,userid),username,MSGCLASS=T,MSGLEVEL=(1,1),
//  NOTIFY = userid
//JOBLIB DD DSN='LL.LOAD',DISP=SHR
//G EXEC PGM=CONV,REGION=95K,TIME=(,20)
//FT05F001 DD DSN=userid.OLDFILE.DATA,DISP=SHR
```



```
//FT06F001 DD SYSOUT=A
//FT07F001 DD DSN=userid.NEWFILE.DATA,DISP=(NEW,CATLG),
//   UNIT=3330-1,VOL=SER=DL0295,SPACE=(TRK,(1,1)),
//   DCB=(RECFM=FB,LRECL=80,BLKSIZE=3120)
//FT08F001 DD DSN=userid.CONFILE.DATA,DISP=SHR
//FT09F001 DD DUMMY
//
```

APPENDIX A

HADES DATASET FORMATS

UCL HADES 3

18A4	Title
18A4	Matrix
either	
8X,3F18.15	3 cards
	Lattice vectors
or	
9X,3(3X,F18.15)	
6X,I5	Number of atoms NAT.
8X,3F18.15,I5	NAT cards. Coordinates and type.
8X,3F18.15	Origin.
6X,I5	Number of vacancies NVAC.
8X,3F18.15,I5	NVAC cards. Vacancy coordinates and type.
6X,I5	Number of interstitials NINT.
8X,3F18.15,I5	NINT cards. Interstitial coordinates and type.
6X,F10.5	Maximum region 2A radius.
18A4	Potential title
6X,I5,10X,F15.5	Number of species NSP and lattice constant
6X,I5,10X,2F15.5	NSP cards. Type, charge, mass
6X,I5,10X,F15.5	Number of potentials, NPOT. Potential cutoff.
6X,2I5,5X,3F15.10	NPOT cards. Potential information
6X,I5,10X,F15.5	Number of spring constants, NSPR. Maximum shell displacement.
6X,2I5,5X,F15.5	NSPR cards. Spring constant data
6X,I5,5(5X,I5)	Number of region 1 sizes. Number of atoms for each size.
6X,F20.10	Region 2 radius (ignored if there is more than 1 region 1 size).

Dataset format 1 has the first format for the lattice vectors, dataset format 4 has the second format.

HADES 2

18A4	Title
6X,3F10.5,I5	3 cards. Lattice vectors
6X,I5	Numer of atomss NAT.
6X,3F10.5,I5	NAT cards. Coordinates and species types. (Cores only)
6X,I5	Number of vacancies NVAC
6X,3F10.5,I5	NVAC cards. Vacancy coordinates
6X,I5	Number of intestitials NINT
6X,3F10.5,I5	NINT cards. Interstitial coordinates and types.
19X,F10.5	Region 2A radius.
6X,I5	Number of region 1 radii. NR1.
6X,I5	NR1 cards. Number of classes in region 1.
6X,I5	Number of lists of potential information. NLIST
18A4	Potential title
6X,F15.5	Lattice constant
6X,I5	Number of ion types NION
6X,I5,5X,3(5X,F10.5)	NION cards. Ion type, ion charge, shell charge, spring constant.
6X,I5,10X,F10.5	NPOT Number of short range potentials. Potential cutoff.
6X,2I5,5X,3(F10.5,5X)	NPOT cards. Number of Potentials.

Repeated from the potential title NLIST times.

ICI HADES 3

L5	Optical switch
18A4	Title
18A4	Matrix
3F20.0	3 cards. Lattice vectors
I10	Number of atoms NAT
3F20.10,I10	NAT cards. Coordinates and types.
3F20.10	Origin
I10	Number of vacancies NVAC
3F20.10,I10	NVAC cards. Vacancy coordinates
I10	Number of interstitials NINT
3F20.10,I10	NINT cards. Interstitial coordinates.
F20.10	Region 2A radius. (This value is ignored)
18A4	Potential title

I10,F20.10		Number of species, lattice constant
I10,2F20.10		NSP cards. Type, charge, mass
I10,F20.10		Number of potentials NPOT. Potential cutoff.
3I10	NPOT	Type I, type J, number of ranges of potential NRANGE.
4F20.10	times	NRANGE cards. Potential data.
		times
I10,F20.10		Number of spring constants, NSPR. Maximum shell displacement.
2I10,F20.10		Species types, Spring constant. NSPR cards
2F20.10		Region 1 and region 2A radii.

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PROGRAM CASCADE.

DESCRIPTION OF DATASETS FOR USE IN CRYSTAL DEFECT CALCULATIONS

by

M. LESLIE, Daresbury Laboratory

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Daresbury Laboratory

Daresbury, Warrington WA4 4AD

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1. INTRODUCTION

This document is a supplement to the previously published description of the input processor for the program CASCADE (Daresbury Laboratory technical memorandum DL/SCI/TM25T, Author: W. Smith). It describes in detail modifications and extensions made since this publication was produced. The major modifications are:

(i) More options for printed output have been added.

(ii) The program will now run PLUTO to relax the strains in the perfect crystal before running the defect calculation.

(iii) The amount of memory required for each job is easily changed. On the CRAY-1 this may be changed at run time without recompiling the program.

(iv) The energies of several defects may be calculated in the same job.

(v) It is possible to restart the job if the time limit or maximum number of iterations are exceeded.

2. OUTPUT OPTIONS

The output options have been modified and extended to give greater flexibility. The PRINT directive now has a format consisting of a number of keywords followed by an integer switch to indicate the level of printing required. In certain cases each digit of the integer is treated as a separate switch for a different part of the program. The IDUMP value is added to the integer (or digit) to increase the amount of output for all of the keywords. A list of the keywords with the possible switch values and the default is given below.

LATT
- 0 No output
- >0 The symmetry matrices of the point group of the lattice vectors are printed.

Default 0.

BASI
- 0 The basis species, defects and origin are output by default.
- >0 The list of basis species is output after sorting into species types and after the shift of origin. The point group matrices of the basis atoms about the specified origin are listed.

The point group matrices of the defect about the origin are listed.

Default 0

REG1 REG2 These switches are both three digit integers where the unit digit refers to the crystal definition phase, the tens digit to the iterative phase and the hundreds digit to the final cycle of the iterative phase. The values of the switches are as follows

0 No output

1 The first ten symmetry classes of each species type are listed.

2 All classes are listed.

3 All members of all classes are listed.

Defaults REG1 202

REG2 101

RECI

0 No output

1 List the first ten reciprocal lattice vectors.

2 List all reciprocal lattice vectors

3 List all symmetry related reciprocal lattice vectors.

Default 2

SYMM

0 No output

1 List symmetry information

Default 0

CLAS

0 No output

1 Output various lists of classes of atoms.

Default 0

PLUT This switch is a five digit integer.

Numbering the digits from right (units digit) to left the digits have the following values and meanings.

Digit 1 0 No output

1 List the basis and bulk strains before the first iteration and after the last iteration of PLUTO

2 List the basis and bulk strains each cycle.

Digit 2 As for digit 1 but listing the elastic constant tensor and dielectric constant tensors.

Digit 3 0 No output

1 List the tensors used in the calculation of region 2 displacements after the last cycle.

Digit 4 0 No output

1 List the force constant matrix before the first cycle and after the last cycle.

2 List the force constant matrix on every cycle of PLUTO.

Digit 5 0 No output

1 List, for each basis atom, the Madelung energy, the short range energy and the contribution to the energy of region 2.

The lattice energy is always listed by default.

Default value 00012

STRU

0 No output

1 Output the structure factors

Default 1

MATR A three digit integer which controls output of the second derivative matrix and its inverse from the defect energy calculation. The units digit refers to the second derivative matrix before inversion, the tens digit to the inverse and the hundreds digit to the updated inverse. The digits may take three values.

0 No output

1 List the gradient vector only

2 List the second derivative matrix or its inverse.

Default 0

ENGY

0 Output only the total defect energy each cycle.

1 Output the various contributions to the defect energy each cycle. Also the interstitial coordinates will be listed each cycle.

Default 0

3. PLUTO ITERATION

An option has been added to CASCADE to allow the user to relax the strains in the lattice before entering the defect energy calculation. Either the positions of the basis atoms in the unit cell or the lattice vectors or both of these may be relaxed to eliminate basls or bulk strains respectively. The iteration is controlled using the START PLUT directive which now has the format

START PLUT int bsinc bkinc litt1 litt2

int is an integer giving the number of times the PLUTO calculation is carried out. (int = 1 therefore does not carry out any iteration). This is the default.

bsinc, bkinc

These are two real numbers giving the factors by which the calcualted displacements are multiplied before updating the position vectors of the basis atoms or the lattice vectors respectively. Values of 0.0 in either field will keep the appropriate vectors fixed.

litt1

is a four character literal which can have the following values.

NONE	No species will be relaxed.
ALL	All species will be relaxed.
CORE	Relax the cores and shells treating the ion as one unit so that no additional core-shell displacements are set up.
SHEL	Relax the shells only keeping the cores fixed.
litt2	is a four character literal which identifies the substance if potentials for more than one substance have been read in. litt2 may be omitted if only one substance is being considered.

If the PLUTO iteration option is selected then the order of the directives in the CASCADE dataset is slightly different to that normally used. The order must now be

LATTICE VECTORS BASIS VECTORS DEFECTS | POTENTIAL INFORMATION | PLUTO | CRYSTAL DEFINITION | RELAXATION

The order normally used is

LATTICE VECTORS BASIS VECTORS DEFECTS | CRYSTAL DEFINITION | POTENTIAL INFORMATION | PLUTO | RELAXATION

If a PLUTO iteration is not carried out either card order is acceptable. It is possible to stop the calculation after the PLUTO phase simply by inserting a STOP directive in the dataset.

Finally, for implementation on the CRAY-1 only, if PLUTO does carry out iterations, the program will attempt to write to FORTRAN unit 8 a list of the updated lattice vectors and basis vectors in a format suitable for inclusion in a CASCADE dataset. Therefore if int is greater than 1, the user must ensure that the CRAY JCL ASSIGN UNIT 8 is used, even if the updated vectors are not required.

This is because the WRITE(8,....) statement will open unit 8 for output and reserve space for the I/O buffers which lies in the space used by the blank common block, and the job will ABORT at a later stage. (See below).

4. ALLOCATION OF MEMORY

Although CASCADE has been written in such a way that it will be possible to implement dynamic core allocation at run time, this has not yet been done. For operation on machines other than the CRAY-1, the integer read in on the DIMENSION card should be the same as the size of the array ISPACE, which is defined in the main segment of the program.

For operation on the CRAY-1, a DIMENSION card is still needed, although the integer value read in has no effect on the running of the program. The user nevertheless does have some control over the size of the program. This is done by requesting a field length for the program using the RFL,M=f1. card in the CRAY JCL. (See CRAY-OS Reference Manual SR-0011 Part 2 2-4.) f1 is an octal integer giving the number of blocks (1000_8 words) into which the program is loaded. The maximum value is 1370. The size of

the blank common block is then determined by reading the relevant constants in the job communication block (see CRAY FORTRAN Reference Manual 2240009 page 3-68.7 and CRAY-OS Reference Manual SR-0011 Apendix A). This array is then used as storage for all the large arrays used by the crystal definition, PLUTO and relaxation sections of the program.

The only difficulty which can arise is that, if a file is opened after the size of the common block has been determined, then space is reserved for the I/O buffers in the upper part of the user field. This may cause the logical file tables (LFT's) to be overwritten and the job to abort. This problem can be avoided by including an ASSIGN card in the CRAY JCL for any FORTRAN unit number to which data may be written or from which data is read. Units 5 and 6 are automatically assigned. The other unit numbers and the circumstances under which they are used are given in Table 1.

TABLE 1

Unit Number	Nature of I/O	Use
7	WRITE (FORMATTED)	Provide a graphics dataset if a PLOT directive is in the CASCADE dataset.
8	WRITE (FORMATTED)	Produce an updated set of lattice and basis vectors from PLUTO. (See part 3 of this manual).
9	WRITE (UNFORMATTED)	Write a relaxed coordinate dump if a WRDU directive is in the CASCADE dataset.
10	READ (UNFORMATTED)	Restart a job from a coordinate dump. (See part 9 of this manual).

If the field length specified is too small, the program will terminate, but it will attempt first to determine the field length needed for the job step in which the run terminated. A successful run will also print the minimum field length needed for the job. This value can then be used if the same or a similar job is run.

5. REGION ONE SIZE SPECIFICATION

The format of the REGI card has been slightly altered. There are now 8 operands instead of 7. The first parameter was the number of classes of atoms required in region 1. This is replaced by two new operands. The first is a four letter keyword and the second is an integer or real variable depending on the keyword. The keywords and variable types needed are

Keyword	Variable Type	Meaning
CLAS	Integer	Number of classes in region 1.
ATOM	Integer	Number of atoms in region 1
RADI	Real	Radius of region 1

If the keyword is omitted the program assumes the CLAS option is being used.

6. RECORD LENGTH SPECIFICATION

Datasets containing standard IBM line numbers (in columns 73-80) may be used. The input processor reads 80 characters per card image, which may lead to problems if the line number is interpreted as data. To avoid this problem a new directive IREC has been implemented. The format is

IREC int

where int is an integer (<80) which specifies the number of characters read in from each record. For a line numbered dataset the directive

IREC 72

should be included either before or after the title.

7. OPTIONS FOR CALCULATING MORE THAN ONE DEFECT ENERGY IN THE SAME JOB

Several options are available to allow the calculation to continue after the first START RELA card. These are

(a) Calculate the defect energy with a new region size.

(b) Calculate the defect energy with a new potential cut-off.

(c) Calculate the energy of the same defect in a different crystal.

(d) Calculate the energy of a different defect in the same crystal.

7(a) NEW REGION SIZE SPECIFICATION

The energy of the defect may be recalculated using a larger region size. The relaxed crystal coordinates may be used as a starting point for the new calculation. In order to re-use the relaxed coordinates a RESTART directive is placed immediately after the START RELA directive. New region sizes must be read in using a REGN diretive which has the format
REGN litt param1 param2.

Litt and param1 specify the new region 1 size as described in Section 5 of this manual. (Litt may be omitted, in which case the CLAS option is assumed). Param2 is the new region 2 radius. Both region sizes must either stay the same or increase. The dataset should then contain a START CRYS and START RELA directive. A typical dataset would be

```
  .
  .
  .
REGI  RADI 1.2 2.4 .....
START CRYS
  .
  .
START RELA
RESTART
REGN  RADI 1.3 2.6
START CRYS
START RELA
  .
  .
```

Convergence in the new region size is usually very rapid, which can result in a considerable saving in CPU time.

7(b) NEW POTENTIAL CUT-OFF

To calculate the defect energy with a new potential cut-off a CUTO directive is used. This has the format CUTO param1 param2 param3 param4

where parameters 1-4 have the following meanings

parameter1	New short range potential cut-off
parameter2	New maximum permissible core-shell separation.
parameter3	New maximum permissible core displacement.
parameter4	New maximum range of potentials.

This is followed by a START PLUT and START RELA directive. The short range potential cut-off should not equal an atom-atom separation in the crystal.

7(c) MORE THAN ONE SUBSTANCE

It is possible to calculate in one job the energies of defects in two or more crystals with the same structure. All the potentials are read in with one call to POTE. It is necessary to specify the lattice constant appropriate to a set of potentials. This is done using a new sub-direction LCON which has the format
LCON litt rlat
where litt is a literal which is used to identify the substance (only the first four characters will be read) and rlat is the lattice constant. The sub-directive LCON must be placed after the species have been read in but before any potentials are read in. The value of LCON read in here overrides that read in on the REGI card. The literal litt must also be supplied on the START PLUT card (see section 3). A maximum of ten lattice constants may be given per run. If the potentials for only one substance are read in, the LCON sub-directive may be omitted. If two substances share a common ion, the potential must be read in twice with a different species label. This is beause the potentials are scaled by the lattice constant to carry out the perfect lattice and defect calculations.

In order to continue the calculation with a new substance it is necessary to re-label the basis species. This is done using the RELB sub-directive in POTE. The RELB card is followed by cards needed to re-label all of the basis atoms. These cards have the format
Oldlabel Newlabel Species (Defect)
where oldlabel is the old species label, e.g. NA+
Newlabel is the new species label e.g. K+
Species is CORE or SHEL

(Defect) is an optional additional parameter (see 7(d) below).

The re-labelling is terminated by an ENDS sub-directive and the potential input routine is then terminated by an additional ENDS card. The directives required after this card are as follows

```
DEFECT
  .
  .
New defect                Optional - Needed if a new defect is defined.
information
  .
  .
ENDS

CUTO                      Optional - needed if the potential cut-off is
                          different.
START  PLUT ..................................  litt.
                          Necessary - litt must agree with the literal
                          given on the LCON directive.
REGN                      Optional - Needed if the crystal regions are
                          changed.
START CRYS                Only needed if there is a new DEFECT or REGN
                          directive.
START RELA
```

An example of a dataset is given below.

```
DIME   180000
CUBI
REGI   RADI   3.0   6.0   2.722   1.5   0.1   1.5   2.0
THERMAL
LATT
1.0    1.0    0.0
1.0    0.0    1.0
0.0    1.0    1.0
BASI
CA2+   CORE   0.0   0.0   0.0
F-     CORE   0.5   0.5   0.5
F-     CORE   0.5   0.5  -0.5
CA2+   SHEL   0.0   0.0   0.0
F-     SHEL   0.5   0.5   0.5
F-     SHEL   0.5   0.5  -0.5
CENTRE        0.5   0.5   0.5
ENDS
DEFECT
F-     CORE   VACA  0.5   0.5   0.5
F-     SHEL   VACA  0.5   0.5   0.5
ENDS
START  CRYS
POTE
SPEC
SR2+   CORE   -3.0378   1.0
CL-    CORE    1.519    1.0
SR2+   SHEL    5.0378   0.0
CL-    SHEL   -2.519    0.0
CA2+   CORE   -3.24     1.0
F-     CORE    1.38     1.0
CA2+   SHEL    5.24     0.0
F-     SHEL   -2.38     0.0
ENDS
LCON   SRCL2   3.588
BUCK   SR2+   SHEL    CL-   SHEL
2250.3      0.3397      0.0      6.0
ENDS
BUCK   CL-    SHEL    CL-   SHEL
1227.18     0.3214      0.0      6.0
ENDS
HARM   SR2+   CORE   SR2+   SHEL   111.9
HARM   CL-    CORE   CL-    SHEL    35.99
LCON   CAF2     2.722
BUCK   CA2+   SHEL   F-     SHEL
1329.6      0.2979      0.0      5.0
ENDS
BUCK   F-     SHEL   F-     SHEL
1808.0      0.293              109.1
```

```
ENDS
HARM   CA2+   CORE   CA2+   SHEL   390.9
HARM   F-     CORE   F-     SHEL   101.2
ENDS
START  PLUT   1      0.0    0.0    NONE   CAF2
START  RELA
POTE
RELB
CA2+   SR2+   CORE
F-     CL-    CORE
CA2+   SR2+   SHEL
F-     CL-    SHEL
ENDS
ENDS
START  PLUT   1      0.0    0.0    NONE   SRCL2
START  RELA
STOP
```

7(d) MORE THAN ONE DEFECT

Two options are available for carrying out such calculations.

Option (i)

This option may be used if it is not necessary to repeat the START CRYS directive. The new defect must have exatly the same unrelaxed co-ordinates as the old defect and the crystal regions for the relaxation will be the same. This option could be used if the energies of several foreign interstitials wre needed. The RELB sub-diretive of POTE is used (see section 7(c)). The RELB card is followed by any number of cards with format

Oldlabel Newlabel Species Defect

The first three parameters have the meanings given in 7(c). Defect is INTE or INTF to indicate that the species is an interstitial. An interstitial which is also an atom of the host lattice can be re-labelled a foreign interstitial in this way without re-labelling the basis atoms. An example of a re-labelling sequence is given below

.
.
.


```
START  RELA
POTE
RELB
FE3+   TI3+   CORE   INTE
FE3+   TI3+   SHEL   INTE
ENDS
ENDS
START  RELA
POTE
RELB
TI3+   MG2+   CORE   INTE
TI3+   MG2+   CORE   INTE
ENDS
ENDS
START  RELA
STOP
```

Option (ii)

In cases other than that described above the user will need a new DEFECT directive and coordinates, a new START CRYS directive and a START RELA directive. The new defect must have the same origin and the same or lower symmetry.

8. COORDINATE DUMP AND RESTART

CASCADE will dump the relaxed coordinates so that a restart may be made under the following circumstances.

i) The jobtime would be exceeded on the next iteration cycle.
ii) The maximum number of iterations is exceeded.
iii) The core shell separation has exceeded the limit set by the REGI directive.
iv) The core displacement for one ion has exceeded the limit set by REGI.

The CRAY JCL necessary to carry out the dump and restart is described in section 10. A dump is written using an unformatted write to FORTRAN unit 9. To obtain a dump a WRDU directive must be included anywhere in

the dataset before the START RELA directive. This will produce a dump even if the job terminates successfully. The dump is read to FORTRAN unit 10. To read a dump file a REDU directive must be placed in the dataset immediately after the DIMENSION directive. The restart dataset must otherwise be exactly the same as that which produced the dump, except that the region sizes may be increased as described in section 7(a).

9. SUMMARY OF CARD ORDER

DIRECTIVE	PREREQUISITE CALL
IREC	
TITL	
DUMP	
PRIN	
MAXI	None - Optional directives
PLOT	
ACCU	
REDU	
WRDU	
DIME	
CUBI or HEXA	
REGI	None - Mandatory directives
OPTI or THER	
LATT	HEXA or CUBI
BASI	LATT, REGI, DIME
DEFE	BASI
POTE	DEFE
PLUT	POTE, THER or OPTI
CRYS	DEFE, PLUT if int > 1
RELA	CRYS, PLUT

After the first call of RELA, the following sequences are possible.

DIRECTIVE	MANDATORY FURTHER DIRECTIVES
RESTART	REGN, CRYS
REGN	CRYS
DEFECT	CRYS
CUTO	PLUTO
POTE-RELB (Interstitials)	None
POTE-RELB (Basis)	PLUTO

10. EXAMPLES OF CRAY JCL

The load module is stored as a permanent dataset on the CRAY disc with a PDN CASCBN under userid LL. The minimum JCL required is given below.

Example 1

```
JOB, JN=useridJOB, US='acct,userid',T=60.
RFL,  M=3D0.
ACCESS, DN=BIN, PDN=CASCBN, ID=LL.
BIN.
/EOF
                                    data
/EOF
/EOJ
```

The RFL control statement is discussed in section 4 of this manual.

The second example gives the JCL needed to write a new set of basis coordinates after the PLUTO iteration has been carried out. The JCL for the PLOT option is similar, although the unit number is FTO7.

Example 2

```
JOB, JN=useridJOB, US='acct,userid', T=60.
ASSIGN, DN=F1, A=FT08.
RFL, M=400.
ACCESS, DN=BIN, PDN=CASCBN, ID=LL.
BIN.
DISPOSE,DN=F1,DC=ST,DF=CB,ID=userid,WAIT, †
```

```
TEXT= 'DSN=userid.PLUOUT.DATA,DISP=(NEW,CATLG)', +
'UNIT=3330-1,VOL=SER=DL0295,SPACE=(TRK(1,1))', +
'DCB=(RECFM=FB,LRECL=80,BLKSIZE=3120)'.
/EOF
                                    data
/EOF
/EOJ
```

The following two examples give the JCL needed to dump the coordinates and to restart after a dump

Example 3: Coordinate dump

```
 10   JOB,JN=useridJOB, US='acct,userid', T=60.
 20   ACCESS,DN=DELETE,PDN=CDUMP,ID=userid,UQ.
 30   DELETE,DN=DELETE.
 40   END.
 50   EXIT.
 60   ASSIGN, DN=C1,A=FT09.
 70   RFL, M=400.
 80   ACCESS,DN=BIN,PDN=CASCBN,ID=LL.
 90   BIN.
100   REWIND,DN=C1.
110   SAVE,DN=C1,PDN=CDUMP,ID=userid.
120   /EOF
```

Lines 20-50 delete an existing permanent dataset called CDUMP (See Daresbury Computer Users Guide, Chapter 10, 10.7 Example 8, Page 41).

Example 4: Restart

```
JOB,JN=useridJOB, US='acct,userid', T=60.
ACCESS,DN=C1,PDN=CDUMP,ID=userid.
ASSIGN,DN=C1,A=FT10.
ACCESS,DN=BIN,PDN=CASCBN,ID=LL.
RFL, M=400.
BIN.
/EOF
```


11. CONVERSION OF HADES DATASETS TO THE CASCADE FORMAT

Introduction

A FORTRAN program has been written to run on the NAS at Daresbury to convert existing datasets to the format needed to run CASCADE. The existing HADES dataset formats are summarised in Appendix A. They will be referred to as HADES III (UCL), HADES II and HADES III (ICI). Before going into detail some general information about the conversion is given below.

(i) Defect Origin

The defect coordinates for a CASCADE dataset are given with respect to the same origin as the basis atoms. For a HADES III dataset the defect coordinates are given with respect to the origin which is read in. The conversion program carries out the necessary subtractions. For a HADES II dataset no origin is read in. The function of the origin is to define the symmetry since the point group is determined by CASCADE and HADES about this point.

(ii) Region Sizes

For HADES III (UCL) up to 5 region 1 sizes may be read in. The conversion program takes the last (largest) of these values for the CASCADE dataset. The region 1 size is defined as the number of species (i.e. cores and shells) in region 1, and the CASCADE dataset is written using the number of atoms option with this value. The region 2 radius is read in twice in the HADES dataset. If there is only one region 1 size given the second value of the region 2 radius is ignored, otherwise it is this value which is used.

For HADES II it is again possible to have more than one region 1 size and again the conversion program takes the last (largest) value. The region 1 size is defined as the number of classes of ions in region 1. This value is doubled to give the number of cores and shells and written to the CASCADE dataset using the number of classes option.

For HADES II (ICI) the region 1 size is read in once only as a radius and written to the CASCADE dataset with the radius option.

(iii) Potential Information

Any species type, potential type or spring constant which is found not to correspond to a basis or interstitial species is ignored.

(iv) Fixed Interstitials

For HADES II datasets only, any interstitial with a negative type number will be marked as a fixed interstitial in the CASCADE dataset.

(v) Specification of more than one Potential

Again only for HADES II, more than one list of potential information may be specified. Any one of these lists may be selected for output.

(vi) Limits on the Array Sizes in the Conversion Program

The maximum number of data cards which may be processed are as follows

BASIS ATOMS	200
VACANCIES	10
INTERSTITIALS	10
SPECIES TYPES	20
POTENTIAL TYPES	20
HARMONIC INTERACTION TYPES	20

(vii) A CRAY END-OF-FILE card (/EOF) and END-OF-JOB card (/EOJ) are written at the end of the CASCADE dataset.

Details of Running the Program

(i) CLIST and JCL needed to run the program

The program is designed to run either interactively or in batch mode. In the interactive mode the program will type questions on the user teletype to which the user responds. In batch mode the responses must be input into a separate dataset which the program can access at run time. The load module is stored in 'LL.LOAD(CONV)'.

(ii) Interactive Mode

A CLIST which will run the program is given below

```
PROC 2 DS1 DS2
FA
FREE F(FT05F001 FT06F001 FT07F001) ATTRLIST(ATTR)
ATTRIB ATTR BLKSIZE(3120) LRECL(80) RECFM(F,B)
ALLOC FILE(FT05F001) DA(&DS1..DATA) SHR
ALLOC FILE(FT06F001) DA(*)
ALLOC FILE(FT07F001) DA(&DS2..DATA) NEW TRACKS-
```



```
 SPACE(1,1) USING(ATTR)
ALLOC FILE(FT08F001) DA(*)
ALLOC FILE(FT09F001) DA(*)
CALL 'LL.LOAD(CONV)'
END
```

If this CLIST is input into a file userid.CLIST(CONVERT) and the user has an existing dataset OLDFILE.DATA then this may be converted to NEWFILE.DATA by typing CONVERT OLDFILE NEWFILE.

USER RESPONSES

After a short while during which the files are allocated the program will begin to type questions on the user terminal. The questions and responses are given below; responses by the user are underlined.

```
TYPE DATASET FORMAT TYPE, I1
1= UCL HADES3, 2 = UCL HADES2, 3 = ICI, 4 = UCL HADES3 NEW
1
FORANT FOR SPECIES LABEL IS 2A4
CHARACTERS 1-4 ARE ION TYPE
EG NA+, CL-, SR2+. THE LABEL MUST NOT CONTAIN ANY SPACES
CHARACTERS 5-8 ARE CORE OR SHEL
TYPE SPECIES LABEL FOR TYPE NO    1
NA+ CORE
TYPE SPECIES LABEL FOR TYPE NO    2
NA+ SHEL
TYPE SPECIES LABEL FOR TYPE NO    3
CL- CORE
TYPE SPECIES LABEL FOR TYPE NO    4
CL- SHEL
TYPE MAXIMUM CORE DISPLACEMENT ALLOWED DURING REFINEMENT, F12.6
2.0
TYPE NUMBER OF TIMES PLUTO CALCULATION IS CARRIED OUT
INCREMENTS ON THE BASIS AND BULK STRAINS PER CYCLE
INCREMENT SWITCH (CORE,SHEL,ALL,NONE)
FORMAT(I4,2F8.4,1X,A4)
   1     0.0     0.0 NONE
TYPE OUTPUT SWITCHES IF DEFAULTS ARE NOT WANTED, OPTIONS ARE
```

```
REG1,REG2,RECI,SYMM,PLUT,CLAS,LATT,BASI,STRU,MATR
FORMAT IS A4,1X,I5, WHERE THE I5 FIELD CONTAINS THE SWITCH VALUE
TERMINATE WITH END
IF NO SWITCHES ARE WANTED JUST TYPE END
ALSO TYPE PLOT IF A PLOT DATASET IS WANTED FROM THE CASCADE RUN
REG1   212
REG2   212
PLOT
END
```

For HADES II datasets the questions and responses are slightly different. After typing the dataset type (2), the questions are

```
THERE ARE     2 LISTS OF POTENTIAL DATA
TYPE WHICH LIST IS REQUIRED, I1
1
FORMAT FOR SPECIES LABEL IS A4
EC NA+, CL-, SR2+. THE LABEL MUST NOT CONTAIN ANY SPACES
TYPE SPECIES LABEL FOR TYPE NO    1
CA2+
TYPE SPECIES LABEL FOR TYPE NO    2
F-
TYPE MAXIMUM ALLOWED CORE-SHELL SEPARATION, F12.6
0.1
```

The questions and responses are then the same starting from TYPE MAXIMUM CORE DISPLACEMENT ALLOWED .....

BATCH MODE

A CNTL file for running the job in batch mode is given below. The user responses given above for the interactive mode are assumed to have been input into the file userid.CONFILE.DATA

```
//useridJOB JOB (acct,userid),username,MSGCLASS=T,MSGLEVEL=(1,1),
//  NOTIFY = userid
//JOBLIB DD DSN='LL.LOAD',DISP=SHR
//G EXEC PGM=CONV,REGION=95K,TIME=(,20)
//FT05F001 DD DSN=userid.OLDFILE.DATA,DISP=SHR
```



```
//FT06F001 DD SYSOUT=A
//FT07F001 DD DSN=userid.NEWFILE.DATA,DISP=(NEW,CATLG),
//   UNIT=3330-1,VOL=SER=0L0295,SPACE=(TRK,(1,1)),
//   DCB=(RECFM=FB,LRECL=80,BLKSIZE=3120)
//FT08F001 DD DSN=userid.CONFILE.DATA,DISP=SHR
//FT09F001 DD DUMMY
//
```

APPENDIX A

HADES DATASET FORMATS

UCL HADES 3

18A4	Title
18A4	Matrix
either	
8X,3F18.15	3 cards
	Lattice vectors
or	
9X,3(3X,F18.15)	
6X,I5	Number of atoms NAT.
8X,3F18.15,I5	NAT cards. Coordinates and type.
8X,3F18.15	Origin.
6X,I5	Number of vacancies NVAC.
8X,3F18.15,I5	NVAC cards. Vacancy coordinates and type.
6X,I5	Number of interstitials NINT.
8X,3F18.15,I5	NINT cards. Interstitial coordinates and type.
6X,F10.5	Maximum region 2A radius.
18A4	Potential title
6X,I5,10X,F15.5	Number of species NSP and lattice constant
6X,I5,10X,2P15.5	NSP cards. Type, charge, mass
6X,I5,10X,F15.5	Number of potentials, NPOT. Potential cutoff.
6X,2I5,5X,3F15.10	NPOT cards. Potential information
6X,I5,10X,F15.5	Number of spring constants, NSPR. Maximum shell displacement.
6X,2I5,5X,F15.5	NSPR cards. Spring constant data
6X,I5,5(5X,I5)	Number of region 1 sizes. Number of atoms for each size.
6X,F20.10	Region 2 radius (ignored if there is more than 1 region 1 size).

Dataset format 1 has the first format for the lattice vectors, dataset format 4 has the second format.

HADES 2

18A4	Title
6X,3F10.5,I5	3 cards. Lattice vectors
6X,I5	Numer of atomss NAT.
6X,3F10.5,I5	NAT cards. Coordinates and species types. (Cores only)
6X,I5	Number of vacancies NVAC
6X,3F10.5,I5	NVAC cards. Vacancy coordinates
6X,I5	Number of intestitials NINT
6X,3F10.5,I5	NINT cards. Interstitial coordinates and types.
19X,F10.5	Region 2A radius.
6X,I5	Number of region 1 radii. NR1.
6X,I5	NR1 cards. Number of classes in region 1.
6X,I5	Number of lists of potential information. NLIST
18A4	Potential title
6X,F15.5	Lattice constant
6X,I5	Number of ion types NION
6X,I5,5X,3(5X,F10.5)	NION cards. Ion type, ion charge, shell charge, spring constant.
6X,I5,10X,F10.5	NPOT Number of short range potentials. Potential cutoff.
6X,2I5,5X,3(F10.5,5X)	NPOT cards. Number of Potentials.

Repeated from the potential title NLIST times.

ICI HADES 3

L5	Optical switch
18A4	Title
18A4	Matrix
3F20.0	3 cards. Lattice vectors
I10	Number of atoms NAT
3F20.10,I10	NAT cards. Coordinates and types.
3F20.10	Origin
I10	Number of vacancies NVAC
3F20.10,I10	NVAC cards. Vacancy coordinates
I10	Number of interstitials NINT
3F20.10,I10	NINT cards. Interstitial coordinates.
F20.10	Region 2A radius. (This value is ignored)
18A4	Potential title

I10,F20.10		Number of species, lattice constant
I10,2F20.10		NSP cards. Type, charge, mass
I10,F20.10		Number of potentials NPOT. Potential cutoff.
3I10	NPOT	Type I, type J, number of ranges of potential NRANGE.
4F20.10	times	NRANGE cards. Potential data.
		times
I10,F20.10		Number of spring constants, NSPR. Maximum shell displacement.
2I10,F20.10		Species types, Spring constant. NSPR cards
2F20.10		Region 1 and region 2A radii.