
DISCUS SUITE

Users Guide

Version 5.23

written by

Reinhard Neder

Email: reinhard.neder@fau.de

<http://tproffen.github.io/DiffuseCode>

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Preface

Disclaimer

The DISCUS SUITE software described in this guide is provided without warranty of any kind. No liability is taken for any loss or damages, direct or indirect, that may result through the use of the DISCUS SUITE. No warranty is made with respect to this manual, or the program and functions therein. There are no warranties that the programs are free of error, or that they are consistent with any standard, or that they will meet the requirement for a particular application. The programs and the manual have been thoroughly checked. Nevertheless, it can not be guaranteed that the manual is correct and up to date in every detail. This manual and the DISCUS SUITE program may be changed without notice.

DISCUS SUITE is intended as a public domain program. It may be used free of charge. Any commercial use is, however, not allowed without permission of the authors.

Using DISCUS SUITE

Publications of results totally or partially obtained using the program DISCUS SUITE should state that DISCUS SUITE was used and contain the following reference:

NEDER, R.B. in preparation - check website.

More information

This users guide can only provide program specific details. A broader discussion of simulation techniques and some DISCUS SUITE examples and macro files can be found in our book

NEDER, R.B. & PROFFEN, TH. "Diffuse Scattering and Defect Structure Simulations - A cook book using the programs DISCUS", *IUCr Texts on Crystallography*, Oxford University Press, 2007.

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Chapter 1

Introduction

1.1 What is DISCUS_SUITE ?

The DISCUS_SUITE is a combination of the components of the DISCUS program suite. It includes the stand alone programs DISCUS, DIFFEV, and KUPLOT under a common command language. The command language is documented in the manual `package_man`.

In this combination, the DISCUS_SUITE allows you to seamlessly switch between the individual sections. Its main advantage lies in the field of massive parallel computing. As the DISCUS_SUITE includes the full functionality of DIFFEV, the DISCUS_SUITE allows you to perform parallel refinements. In contrast to a stand alone DIFFEV, the DISCUS_SUITE does have to perform nearly no I/O during the refinement.

See the DIFFEV manual for full details of the refinement process.

1.2 Getting started

1.2.1 Windows

Once the programs have been installed you should see an icon for each of the programs on your personal desktop. Double click the icon to start the program of your choice.

At program start, each of the programs sets its starting folder to

```
C:\Users\your_name
```

where `your_name` will be your user name. The string `Users` may be slightly different depending on the language settings. To work with data and macros that are stored in a separate folder, you need to change to this folder.

Within the DIFFUSE program window, type the command `cd` including a blank space after the `cd`. At this point do not hit the enter key. Open the desired folder with the Windows-Explorer. Left click on the small folder symbol in the top line that indicates the path to your folder. This should highlight the full path to the folder.

For DISCUS, DIFFEV, you can drag this folder symbol into the DIFFUSE program window. The command line should now read something like

```
cd C:\Users\Neder\Documents\DISCUS_examples
```

For KUPLOT and DISCUS SUITE, select the highlighted path to the folder with CTRL-c. Activate the KUPLOT or DISCUS SUITE window and press the middle button on the mouse. This should place the full path into the program window.

Once you activate the window and hit the ENTER key the program will work in this folder.

1.2.2 Linux

After the program *DISCUS_SUITE* has been installed properly and the environment variables are set, the program can be started by typing 'discus_suite' at the operating systems prompt.

Symbol	Description
"text"	Text given in double quotes is to be understood as typed.
<text>	Text given in angled brackets is to be replaced by an appropriate value, if the corresponding line is used in DISCUS SUITE. It could, for example be the actual name of a file, or a numerical value.
text	Text in single quotes exclusively refers to DISCUS SUITE commands.
[text]	Text in square brackets describes an optional parameter or command. If omitted, a default value is used, else the complete text given in the square brackets is to be typed.
{text text}	Text given in curly brackets is a list of alternative parameters. A vertical line separates two alternative, mutually exclusive parameters.

Table 1.1: Used symbols

The program uses a command language to interact with the user. The command `exit` terminates the program and returns control to the shell. All commands of DISCUS SUITE consist of a command verb, optionally followed by one or more parameters. All parameters must be separated from one another by a comma ",". There is no predefined need for any specific sequence of commands. DISCUS SUITE is case sensitive, all commands and alphabetic parameters MUST be typed in lower case letters. If DISCUS SUITE has been compiled using the `-DREADLINE` option (see installation files) basic line editing and recall of commands is possible. For more information refer to the reference manual or check the online help using (`help command input`). Names of input or output files are to be typed as they will be expected by the shell. If necessary include a path to the file. All commands may be abbreviated to the shortest unique possibility. At least a single space is needed between the command verb and the first parameter. No comma is to precede the first parameter. A line can be marked as comment by inserting a "#" as first character in the line.

The symbols used throughout this manual to describe commands, command parameters, or explicit text used by the program DISCUS SUITE are listed in Table 1.1. There are several sources of information, first DISCUS SUITE has a build in online help, which can be accessed by entering the command `help` or if help for a particular command `<cmd>` is wanted by `help <cmd>`. This manual describes background and principle functions of DISCUS SUITE and should give some insight in the ways to use this program.

DISCUS SUITE is distributed as part of the diffuse scattering simulation software DISCUS. In contrast to, DIFFEV, DISCUS SUITE does not lend itself as efficiently as a general refinement

program separate from the DISCUS program package. DISCUS SUITE handles a structure refinement via the internal DISCUS and KUPLOT sections.

Command line options

Several command line options are available for the Linux version. The most important one is to start the execution of a macro:

```
discus_suite -macro useful.mac  
discus_suite -macro useful_with_params.mac par1 par2 par3
```

The first line would start DISCUS SUITE and begin the automatic execution of macro `useful.mac`. Likewise in the second line, the macro `useful_with_params.mac` is started, which takes three parameters. The actual strings that you provide for `par1`, `par2`, `par3` are handed down as parameters to this macro. Note that there are no comma between the parameters. For info on further command line options the on-line help for the Command language.

1.3 Parallel execution

The typical application of the DISCUS SUITE is a run on a massive parallel system. You will have to check for details with your local administrator. In general you should expect to start DISCUS SUITE along the lines of:

```
mpiexec -n 192 discus_suite -macro refine.mac > /dev/null
```

The command `mpiexec` initiates the MPI system. Here in this example we request 192 CPUs `-n 192`. The MPI system then starts the DISCUS SUITE and read its input from the macro `refine.mac`. All output is discarded to `/dev/null` in order to minimize I/O. During development of your macro you might redirect the output to a logfile.

The example line above works fine on a single multi-core computer with Linux. The number of processes would be more reasonably placed around the number of CPUs on your computer. Within the Windows version, parallel execution of such a macro is performed by DISCUS SUITE command *parallel*:

```
parallel refine.mac  
parallel 6, refine.mac
```

The first command version instructs DISCUS SUITE to run a parallel refinement via the macro *suite.mac*. The number of parallel threads is determined automatically. Alternatively you can tell DISCUS SUITE how many parallel threads you would like to run by adding the number of threads prior to the macro name. In the example above DISCUS SUITE is instructed to use 6 threads.

1.4 Command language

The program includes a FORTRAN style interpreter that allows the user to program complex modifications. A detailed discussion about the command language which is common to all DISCUS package programs can be found in the separate package reference guide which is included with the package. At the moment, DISCUS SUITE does not include any specific variables.

Chapter 2

Concepts

2.1 Quick overview

The purpose of the DISCUS SUITE is to run a combination of DIFFEV, DISCUS, and KUPLOT within a single program. The DISCUS SUITE should for all practical reasons be the main program you start. Its main application will be a run on a massive parallel system, but it will already pose an improvement on a multi-core laptop. DISCUS SUITE uses MPI to distribute a part of its workload onto several processes. The original DIFFEV starts DISCUS as a separate slave program. This means that at each refinement cycle DISCUS has to read all macros, and other relevant information over and over again. This causes a lot of unnecessary I/O, which puts a considerable burden onto the central disk system.

As DISCUS SUITE includes DIFFEV, DISCUS, and KUPLOT within one single program, all relevant input can be read once at the beginning of the refinement cycle. It will from there on be kept in internal memory, thus eliminating the need of further input. This includes the trial parameters as well as the result values. In the stand alone program DIFFEV, these values are passed from DIFFEV to and forth between DISCUS and KUPLOT via (small) files on the disk. Within DISCUS SUITE, the need to write these files onto the disk no longer exists and DISCUS SUITE instructs DIFFEV to store these values only internally.

As the main tasks are still performed within the sections DIFFEV, DISCUS, and KUPLOT, the actual set of commands within DISCUS SUITE is very limited. Besides the general command of the common command language the commands are just the names of the three sections, Table 2.1.

Within the three sections, a few details are slightly different compared to their stand alone

Command	Description
diffev	Switch to the <code>diffev</code> section. in many cases this will be the only command used within the top menu of the suite.
discus	Switch to the <code>discus</code> section.
kuplot	Switch to the <code>kuplot</code> section.
parallel	Run a parallel refinement.

Table 2.1: DISCUS SUITE command verbs.

versions. The main command syntax and typical command sequences are, however, identical. As DISCUS SUITE is a single program, the global variables `i[]`, `r[]`, `res[]` are identical throughout all sections. The same holds for user defined variables. Thus, for example, if `i[0]` is set to one value in any section, all other sections will see this new value. Be careful when you combine old DISCUS and KUPLOT macros. Their local variables may interfere with each other. Besides the three variables `i[]`, `r[]`, `res[]` and the user defined variables, each of the three sections includes specific variables that are valid and meaningful within this section only. These variables specific to any of the sections are visible within that section only.

2.2 Modified concepts

In order to fully utilize the common program architecture, a few details should be used in a modified way within the different sections. These details mostly concern disk I/O related parts.

2.2.1 DIFFEV

The stand alone DIFFEV communicates with DISCUS and KUPLOT via (small) files that contain the trial parameters and the cost function results. To avoid writing these to disk use:

```
init silent
```

The new `silent` parameter tells the DIFFEV section with the DISCUS SUITE not to write an initial set of trial parameters to disk. These values are automatically transferred to the slave sections.

Closely related is the modified command:

```
trialfile silent
```

which likewise tells DIFFEV not to write trial files during the refinement cycles.

In both cases the DISCUS SUITE will use the internal variables to communicate the trial parameters to the slave sections. The trial parameters are set up within DIFFEV as variable names and can be referenced with these names within the other sections. Likewise, the information on the current generation is transferred with special variable names. See the DIFFEV manual for full details.

As an example, to define the *a* and *c* lattice parameters for a Wurtzite type structure use the commands:

```
newpara P_lata, 3.85, 3.95, 3.88, 3.92
newpara P_latc, 6.45, 6.55, 6.48, 6.52
```

See the chapter Example in the DIFFEV manual for a fully documented example. The remainder of this section is obsolete for versions 5.22 and later.

For backwards compatibility the variables `ref_para[entry_number]` are retained. Entries in this array range from 1 to the number of parameters to be refined, as defined by `tt pop_dimx` in DIFFEV. As of Versions 5.7 the data are still written to the array, `r` as well. As a deliberate break compared to the general flexibility in all DISCUS SUITE sections, the trial values are stored in entries starting at `r[201]`. Use of these entries is meant to preserve backwards compatibility but will be discontinued in future releases.

Another predefined section of the internal variables is the range:

Entry	Description
i[201]	Current generation number
i[202]	Size of the population
i[203]	Size of the child population
i[204]	Number of parameters

The use of this predefined section of the internal variables is discouraged and has been replaced by the variables:

Entry	Description
REF_GENERATION	Current generation number
REF_MEMBER	Size of the population
REF_CHILDREN	Size of the child population
REF_DIMENSION	Number of parameters
REF_KID	Current child to work on
REF_INDIV	Current individual repetition of the current child

To retain the backwards compatibility, the actual child number and the number of the individual repetition are transferred as parameters on the `run_mpi` command line.

In the DISCUS SUITE version of KUPLOT, a new internal variable is used to store and transfer the weighted R-value from KUPLOT to DIFFEV. Thus, the need to write and read the result file ceases to exist. Do this via the commands:

```
resultfile silent
...           ! further initialization
run_mpi ...   ! Calculate with Discus and Kuplot
compare silent
```

The first and last lines instruct the DIFFEV section not to read the resultfile but to use the value that is transferred internally.

MPI has been implemented in the current Windows installation as well starting with Version 5.7. Use the icon `DISCUS_Suite Parallel_Version` for parallel refinements.

Even in the single session version of the DISCUS SUITE, the refinement should use the `run_mpi` command in an identical fashion.

In order to use the suite efficiently, the `branch` command is available within DIFFEV as well, and you can branch to either DISCUS or KUPLOT. This command should replace the `system discus < discus_macro_name` construction that is used in a serial refinement set up:

```
1  diffev
2  ... SETUP ...
3  init silent
4  branch discus
5  @discus_macro.mac
6  exit
7  branch kuplot
8  @kuplot_macro.mac
9  exit
10 compare silent
11 exit
```

In this simplified example, we switch to the diffev section with the `diffev` command in line 1. After initial setup done by DIFFEV and the initialization of generation zero in line 3, the

DIFFEV section branches off to the DISCUS section in line 4. Now control is at DISCUS and the loop over all children and all calculations are performed by the macro `diffdev_macro.mac` in line 5. The `exit` command in line 5 returns to the DIFFEV section. If you use a previous DISCUS macro, the `exit` line might be part of the DISCUS macro! Lines 7 to 9 do the same for KUPLOT. The `compare` command (line 10) at the DIFFEV level does the comparison between the generations, and finally we leave the DIFFEV section in line 11. In a full refinement there would be a loop over all refinement cycles that includes lines 4 to 10 of this example.

2.2.2 DISCUS

The performance of DISCUS is not directly affected by the DISCUS SUITE. To make full use of the DISCUS SUITE, a couple of concepts should be adhered to.

Use the trial parameter value through the variable names that are defined within DIFFEV. Use the variables `REF_GENERATION`, `REF_MEMBER`, `REF_CHILDREN`, `REF_KID`, `REF_INDIV` to obtain the current generation number, the size of the population, the number of children and the number of trial parameters. Do not open and read the file `GENERATION`. This file is created within each refinement cycle, and has been augmented by a lot of information that DIFFEV reads to continue an interrupted refinement. Within the sections DISCUS and KUPLOT there is, however, no longer any need to read it.

If the initial asymmetric unit is not extremely long, it is best to build the initial asymmetric unit from scratch. To build a Wurtzite type asymmetric unit use the following command sequence:

```
1  read
2  free P_lata, P_lata, P_latc, 90.00, 90.00, 120.00, P63mc
3  insert Zn, 1./3., 2./3, P_zn_z, P-biso
4  insert S , 1./3., 2./3, 0.00 , P-biso
5  save
6  outf internal.wurtzite.cell
7  omit all
8  write scat
9  write adp
10 run
11 exit
12 read
13 cell internal.wurtzite.cell, 5,5,5
```

In this example it is assumed that `P_lata` contains the a lattice parameter value, `P_latc` the c lattice parameter, `P_zn_z` the z-position of Zn and `P_biso` a common atomic displacement parameter B. The last parameter in line 2 tells DISCUS that the structure belongs to space group P63mc. The asymmetric unit is stored internally into computer memory in lines 5 to 11, and then expanded into a block of 5x5x5 unit cells in lines 12 and 13. By providing the space group symbol as last parameter to the `free` command, the expansion in line 13 will ensure that the two atoms Zn and O are properly copied to create all atoms in the unit cell. This macro section does not perform any disk I/O and will be much more efficient on a large parallel system.

Do use the internal storage whenever you need to save a temporary crystal structure. Every time a file name is preceded with the string `internal`, DISCUS will save / read the structure to / from internal memory.

To perform any further manipulations with the calculated data like multiplication by a scale factor, the addition of a background etc., KUPLOT needs to be executed once the DISCUS section is finished. To allow efficient use of massive parallel systems the new `branch` command has

been added to DISCUS and KUPLOT. It allows to switch directly from the DISCUS section to the KUPLOT section within DISCUS SUITE.

```

0  ...                               ! Discus initialization
1  do indiv=1,nindiv                 ! Repeat nanoparticle generation nindiv times
2    @discus.zno.mac kid             ! do the actual simulation
3  enddo
4  branch kuplot                     ! Switch to KUPLOT
5    @kup.diffov.mac ., kid          ! Contains a final exit
6  exit                             ! Finish DISCUS

```

In this DISCUS macro section the simulation of nanoparticles is repeated several (nindiv) times. This might be necessary to average out the defect distribution within the nanoparticles. Under these circumstances the individual calculated diffraction pattern / PDFs need to be averaged after the DISCUS section is finished. The branch to the KUPLOT section in line 4 allows DISCUS to do this while remaining on the identical slave process and thus on the identical compute node. On many massive parallel systems data transfer from a compute node to the central disk is time consuming and many of these systems have local fast (RAM) disks. The DISCUS section can write the individual diffraction pattern / PDF to this local disk without much of a penalty. But then, KUPLOT needs to operate on the same node in order to find the data. This is ensured by the branch construct.

In the alternative set up :

```

0  ...                               ! Diffov initialization
1  run\_mpi discus, discus\_macro.mac " Discus calculation
2  run\_mpi kuplot, kuplot\_macro.mac ! Kuplot calculation

```

DIFFEV will distribute the DISCUS jobs onto all nodes, and then do the same with the KUPLOT jobs. As of version 5.18 the DISCUS SUITE will ensure taht the two jobs for a given child are performed on the identical node.

2.2.3 KUPLOT

In the same fashion as DISCUS , the KUPLOT section should rely on the variables `ref_para[]` `REF_GENERATION` `REF_MEMBER`, `REF_CHILDREN`, `REF_KID`, `ref_INDIV` to determine the population size and if necessary the trial parameters. Do not read the GENERATION file.

Do not write a result file. The KUPLOT instruction:

```
rvalue 1, 2
```

stores the weighted R-value internally and instructs the DISCUS SUITE to transfer the value from the slave process back to the master process. The master process can then use this in the `compare silent` command.

The `branch` command is available within KUPLOT as well, and you can branch to either DIFFEV or DISCUS . Most application will probably not need to do this.

Appendix A

SUITE commands

A.1 Summary

You can switch to the individual sections "discus", "diffv", and "kuplot" by typing the respective section name. To return to the suite type "exit" at the main menu of each section.

The variables i[*], r[*] and res[*] are global variables, a change in any section will be seen in any other section as well. The same holds for all user defined variables!

The section specific variables are local within each section.

If an output filename in "discus" starts with "kuplot", the data are written directly into the next available KUPLOT data set. This is available for Fourier output, powder, pdf.

A.2 News

2018_June

Revised the reaction to a CTRL-C

Added a ==> 'set error, ... , "save" option

2018_Jan

The logical comparisons may now take the operators: <, <=, ==, /=, >=, >/ The classical fortran77 operators are still valid

New logical functions "isvar" and "isexp" can be used within an "if" construction. See help entry ==>'function' in the general "Command_lang" section

2017_Sep

Throughout the program the internal calculation of random numbers was changed to the FORTRAN 90 intrinsic function.

2016_Dec

At a few select points colors are introduced into the output. Currently these are just the error messages.

2016_Oct

A new command 'parallel' has been added to the Windows version This allows to execute a macro in parallel.

2016_June

The SUITE may now be interrupted gracefully with a CTRL-c. This will cause the DISCUS part to write the current structure, and DIFFEV to shut down MPI if active.

2015_December

The branch command within the sections discuss, diffev, kuplot may now take the form : branch discuss -macro macro_name par1, par2, ...

2015_June

Starting with Version 5.1, we have migrated to a X-Window environment for WINDOWS as well. As a small side effect, the technique to jump to the desired folder has changed slightly. See the help entry on "cd" in the general "Command_lang" section for further information. The process is described in the package manual as well.

A.3 diffev

Switches to the "diffev" section.

Within this section any standard DIFFEV command can be given. The behaviour of "diffev" is essentially the same as in the stand alone version. The 'diffev/run_mpi' command will start a discuss/kuplot section. The syntax of the command is unchanged. All trial parameters are placed into array <r[]> at entries 201, 202, ... The values of generation, member, children and number of parameters are placed into <i[]>: i[201] = generation i[202] = member i[203] = children i[204] = parameter

Use an 'exit' to return to the suite.

A.4 discuss

Switches to the "discuss" section.

Within this section any standard DISCUS command can be given. The behaviour of "discuss" is essentially the same as in the stand alone version.

Within the discuss section you can use the command 'branch kuplot' to switch to the kuplot branch.

In contrast to the stand alone DISCUS version, one can write an output file directly into the KUPLOT data sets. The number of data sets in KUPLOT is automatically incremented. Currently this is implemented for the PDF and the powder output. Single crystal diffraction pattern to follow shortly.

A.5 kuplot

Switches to the "kuplot" section.

Within this section any standard KUPLOT command can be given. The behaviour of "kuplot" is essentially the same as in the stand alone version.

Within the kuplot section you can use the command 'branch discus' to switch to the discus branch.

A.6 parallel

parallel {<numprocs>, },<macro.mac> {, <para_1...}

Starts an MPI driven parallel calculation. See the diffev help on a full explanation of parallel processing.

The parallel refinement will execute file <macro.mac>, which must reside in the current directory. Make sure you have used `cd <path>` to change to the proper directory prior to the use of the 'parallel' command. The macro name must be given in full, including the ".mac" extension. If the macro requires parameters you must specify these following the macro name.

Optionally you can place the number of processes that MPI shall start prior to the macro name. The numebr defaults to the value of the SHELL variable `NUMBER_OF_PROCESSORS` on your system. If this variable is not set, discus_suite will start 4 processes.

A.7 manual

manual ["section:"{"suite" | "discus" | "diffev" |
"kuplot" | "package" | "mixscat"}
[, "viewer:"<name>]

Opens a PDF viewer for one of the Manuals

The section defaults to the current program section that you are working with. On Linux systems, the viewer defaults to "qpdfview", on Windows system it defaults to "firefox". If DISCUS does not find the default or the user provided viewer, DISCUS will search a list of common PDF viewers. If none is found an error message points to the folder that contains the manuals.

Bibliography