Package name: EPRSIM C – technical information

Program name: EPRSIM BBW

Icon:

OS environment: MS Windows (32 bit)
Console application

Version & Release: 6.2.5

Purpose:
- automatic optimization,
- multithreading,
- multiple spectra optimization,
- background calculation,
- single run / stay-resident /cluster mode
- automatic start

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1   EPRSIM BBW usage

1.1 EPRSIM BBW Modes

EPRSIM BBW is designed as numerical intensive part of EPRSIM C software package as a console application. Its function is optimization of spectral parameters / spectral fitting. However, it can be used in the following ways:

Mode A – independent application / single MTP optimization
Mode B – stay-resident application
Mode C – numerical-intensive cluster module (high-end)

Different modes are triggered via various switches in command prompt where EPRSIM BBW is run from.

1.2 EPRSIM BBW switches

1.2.1 Main switches:

-p=*mtpfilename* … initiation of BBW in mode A – starting optimization for problems defined in MTP file with filename *mtpfilename*; note that the appropriate spectral files should be in the same folder as MTP files;

-d=*directoryname* … initiation of BBW in mode B – stay-resident mode; BBW will check directory with directory name *directoryname* every 30 seconds in order to find MTP file (with problems not yet solved) and start optimizations; the same directory is searched for new/other MTP files when one MTP is finished; the directory can be located on a local computer or elsewhere in local Microsoft network;

-c=*masterIPaddress* … initiation of BBW in mode C – cluster mode; *masterIPaddress* represents IP address of the computer where Master is located to establish functional connection with Master;

1.2.2 Additional switches:

-n=*numberofthreads* … *numberofthreads* is maximal number of working threads allowed in BBW; recommended number of threads equals the number of processors on certain computer; used in all modes;

-k=*numberofcopies* … *numberofcopies* is number of independent optimizations that should be run on each problem defined in MTP file – can be override by the definition inside MTP file; rarely used in all modes;

-s=*speedindex* … *speedindex* indicates relative speed of the certain computer when connecting in cluster mode for efficient load balancing; natural unit of *speedindex* is MFLOPS, but can be anything; used only in cluster mode (mode C)

1.2.3 Examples of program evaluation:

1. To run EPRSIM BBW in <u>mode A (single MTP optimization)</u>, pointing to the »c:\temp\test.mtp« file containing problems for optimization, allowing at maximum 2 parallel threads and forcing 20 independent runs on each problem defined in MTP file, one should input the following line:

   eprsimbbw.exe -p=c:\temp\test.mtp -n=2 -k=20

   When the optimization is finished, the optimized results are written in terms of "test1.mtp" file containing best fits, and POP subdirectory containing population files for GHOST construction, and EPRSIM BBW program terminates.

2. To run EPRSIM BBW in <u>mode B (stay-resident)</u>, pointing to the »c:\temp« directory that eventually contains MTP files with problems for optimization, allowing at maximum 2 parallel threads and forcing 20 independent runs on each problem defined in MTP file, one should input the following line:

   eprsimbbw.exe -d=c:\temp -n=2 -k=20

   After EPRSIM BBW is started, it checks the »c:\temp« directory every 30 second for new MTP files to start optimization. When MTP file (together with appropriate spectral data files) is copied to »c:\temp« directory, EPRSIM BBW will automatically start optimization at lately in 30 seconds. When finished, it starts to scan the directory again.

   EPRSIM BBW can be started directly from command line (prompt) or from Windows Schedule to enable pure background running.

   EPRSIM BBW can be terminated through Task Manager or Windows Schedule (if used).

   File transfer to the directory can be from anywhere (with appropriate permissions) through the local network. When several new MTP files are found in the directory, the oldest one starts first.

   Note, that after the task is finished and all the results in terms of MTP files and POP subdirectories, one has to copy these results to the local folders. Not to crash EPRSIM BBW due to slow copying it is recommended to do this in the following order:
   - first move the MTP files
   - second move the spectral files and delete messages (exceptions) if not needed
   - third move appropriate POP directory
   Do NOT try to move or open MTP files that are in use.

3. To run EPRSIM BBW in <u>mode C (cluster)</u>, pointing to the master computer with IP address of 201.2.16.240, allowing at maximum 2 parallel threads, defining the speed of the local computer to be of 2000, one should input the following line:

   eprsimbbw.exe -c=201.2.16.240 -n=2 -s=2000

After EPRSIM BBW is started in cluster mode, it tries to open the connection to the EPRSIM Master at the master computer indicated by IP address of 201.2.16.240. The master put the local computer on the list, which is used to send optimizations jobs. The jobs are sent to the fastest computer available at the moment. EPRSIM BBW can be terminated through Task Manager.

2   EPRSIM BBW input/output

2.1 Input - MTP file format

The main format of data used by EPRSIM C package is MTP file format. It is text format, including 2 block of information.

Block A – program constants and parameters
Block B – multiple-block with problem specific constants and parameters

An example of typical structure of MTP file that includes Block A and 2 problems defined Block B is explained below.

IMPORTANT: Notes indicated with red color should not be included in regular MTP file! Real content of the MTP file is indicated by the vertical bar on the left.

```
Begin of Block A:

(g and A tensor components & C13 A scalar coupling & C13 abundance – CHOOSE THE
CORRECT TENSORS VALUES !!!!)
Tensors:
2.0090 2.0063 2.0026 6.500 5.500 34.100 5.600 0.0115
(Additional Gaussian noise that should be added to experimental spectra;
relative units of 1; default value should be 0.5 % to allow simplex downhill to
converge for any spectral type)
Noise:
0.005
(do not change – kept for compatibility with older software)
Asimetric distribution:
1.00 0.0000
(lower and upper limits of spectral parameters for all spectral models built in
EPRSIM C)
Limits:
(1st model: isotropic tumbling = ISO – proportion of Lorentzian/Gaussian
mixture, isotropic rotational correlation time in ns, additional broadening
constant in G, polarity correction pA, polarity correction pg, weight)
0.000 1.000 0.010 1.000 0.100 1.000 0.8000 1.2000 0.999600 1.000400 0.010 0.990
(2nd model: anisotropic tumbling with full averaging over other axes = MEM –
order parameter Szz, isotropic rotational correlation time in ns, additional
broadening constant in G, polarity correction pA, polarity correction pg,
weight)
0.020 1.000 0.100 3.000 0.200 4.000 0.8000 1.2000 0.999600 1.000400 0.010 0.990
(3rd model: isotropic spin-exchange label-label = LLE – isotropic rotational
correlation time in ns, additional broadening constant in G (not originating
from spin-exchange), spin exchange rate in G, polarity correction pA, polarity
correction pg, weight)
0.100 3.000 0.100 1.500 0.000 10.000 0.8000 1.2000 0.999600 1.000400 0.010 0.990
(4rd model: isotropic spin-exchange label-broadening agent = LBE – isotropic
rotational correlation time in ns, intrinsic linewidth of broadening agent in G,
concentration of broadening agent in mmol/l, additional broadening constant in G
(not originating from spin-exchange), spin exchange rate in G, polarity
correction pA, polarity correction pg, weight)
```

```
0.100 3.000 100.000 3000.000 100.000 10000.000 0.100 1.500 0.000 15.000 0.8000
1.2000 0.999600 1.000400 0.010 0.990
```
```
0.01 0.99 0.00 1.57 0.00 1.57 0.00 1.57 0.00 1.57 0.00 1.57 0.100 3.000 0.200
4.000 0.8000 1.2000 -0.070 0.070 0.010 0.990
```
```
0.00 0.30 0.10 1.57 0.10 1.57 0.100 1.570 0.000 20.000 0.1000 10.0000 0.200000
4.000000 0.800 1.200
```
```
0.01 0.99 0.00 1.57 0.00 1.57 0.00 1.57 0.00 15.00 0.00 15.00 0.00 15.00 0.100
10.000 0.200 4.000 0.8000 1.2000 0.999600 1.000400 0.010 0.990
```
```
0.00 10.00 0.00 1.57 0.00 1.57 0.00 1.57 0.00 15.00 0.00 15.00 0.00 15.00 0.100
10.000 0.200 4.000 0.8000 1.2000 0.999600 1.000400 0.010 0.990
```
```
0.000 1.000 0.050 3.000 0.999600 1.000400 0.00 5.00 0.0 10.0 0.0000 50.0000 0.00
5.00 0.0 10.0 0.0000 50.0000 0.00 5.00 0.0 10.0 0.0000 50.0000 0.00 5.00 0.0
10.0 0.0000 50.0000 0.00 5.00 0.0 10.0 0.0000 50.0000 0.010 0.990
```
```
Grids:
0.020 0.050 0.050 0.0010 0.000002 0.001
0.005 0.050 0.050 0.0010 0.000002 0.005
0.050 0.050 0.100 0.0050 0.000005 0.010
0.050 100.000 100.000 0.050 0.100 0.0050 0.000005 0.010
0.02 0.05 0.02 0.05 0.05 0.05 0.050 0.050 0.0010 0.002 0.005
0.02 0.02 0.02 0.020 0.050 0.0500 0.050000 0.001
0.02 0.05 0.02 0.05 0.05 0.05 0.05 0.050 0.050 0.0010 0.000002 0.005
0.10 0.05 0.02 0.05 0.05 0.05 0.05 0.050 0.050 0.0010 0.000002 0.005
0.020 0.050 0.000002 0.50 1.0 0.0100 0.50 1.0 0.0100 0.50 1.0 0.0100 0.50 1.0
0.0100 0.50 1.0 0.0100 0.001
```
```
Optimization used:
HEA
```
```
Downhill Simplex:
0.10
55
```
```
Hybrid Evolutionary Algorithm:
200
0.050
TRUE
```
```
  Elite
TRUE
0.020
```
```
  Crossover
0.700
MP
0.5
3
```
```
  Hybridization with DS during HEA
TRUE
0.002
  Hybridization with DS after HEA
FALSE
```

0.10
(HEO constants – hybrid: usage of knowledge-based operators: tc-d equilibrator
with probability, W-d equilibrator with probability, polarity sorter with
probability – if model 5 is used polarity sorter should be switched off)
   knowledge-based operators
TRUE
0.100
TRUE
0.100
FALSE
0.100
(other constants: do not change)
Multiple:
FALSE
FALSE
Error analysis:
0
TRUE
TRUE

(MTP number of copies – in this case 20 – number of independent optimizations
that should be run on each problem defined in this file – this definition
replace switch which is used as an external parameter from command line call)
Number of copies:
20
End of Block A

Begin of Block B :
(An example of problem definition 1:)
Spectrum characteristics-1:
(described by 1 experimental file, put up to 5 if more frequencies or angles are
applied)
1
(filenames of all experimental files for this problem)
C:\Documents and Settings\Guest\PM2V137.SPC
(center field, sweep, frequency and angle for each experimental file)
3425.390 100.00 9.61461 0.000
(data about domain parameters)
Domains - types, parameters, errors, switches, group number:
(number of domains, i.e. spectral components)
4
(domain parameters: index of domain, fixed parameter – do not change, type of
model, parameters – see definition above; use the following values according to
model when sent to automatic optimization:
iso 0.2 1 1 1 1 1
mem 0.5 1 1 1 1 1
lle 0.5 1 1 1 1 1
lbe 0.5 100 1800 1 0 1 1 1
mes –1 0 0 0 0.2 1 1 1 1 0 1
psd 0 1.000 0.100 1.570 1 1 1 1 1 1
oms 0 0 0 0 3 0 0 1 1 1 1 1
obs 0.25 0 0 0 3 0 0 1 1 1 1 1
trp 0.2 1 1 1 1 15 0.5 1 2 0 0 1 0 0 1 0 0 1 1)
1 2 mes –1.00 0.00 0.00 0.00 1.08 1.07 1.062 0.897 1.0006 0.009 0.192
2 2 mes –1.00 0.00 0.00 0.00 1.09 1.07 0.845 0.860 0.9969 –0.031 0.242
3 2 mes –1.00 0.00 0.00 0.00 1.29 1.29 1.108 0.944 0.9966 –0.007 0.262
4 2 mes –1.00 0.00 0.00 0.00 1.56 1.43 1.042 0.704 1.0001 –0.004 0.305
(domain parameters' errors: index of domain, fixed parameter – do not change,
type of model, parameters' errors)
1 2 mes 0.00 0.00 0.00 0.00 0.31 0.30 2.535 1.528 0.0692 0.000 0.000
2 2 mes 0.00 0.00 0.00 0.00 0.17 0.17 0.961 1.133 0.0386 0.000 0.000
3 2 mes 0.00 0.00 0.00 0.00 0.06 0.07 0.788 0.333 0.0151 0.029 0.052
4 2 mes 0.00 0.00 0.00 0.00 0.00 0.00 0.169 0.110 0.0041 0.010 0.052
(domain parameters switches: index of domain, fixed parameter – do not change,
type of model, parameters' switches; use the following values according to model
when sent to automatic optimization; last switch (last weight) should be always
false:
iso T T T T T T
mem T T T T T T
lle T T T T T T
lbe T F F T T T T T
mes F F F F T T T T T T T
psd T T T T T T T T T T
oms F F F F T T T T T T T T
obs T F F F T T T T T T T T
trp T T T F T T F T T F T T F T T F T T T)
1 2 mes F F F F T T T T T T T

```
2 2 mes F F F F T T T T T T T
3 2 mes F F F F T T T T T T T
4 2 mes F F F F T T T T T T F
(group number - grouping index can be used to group lately the results of
multiple optimization)
1
(type of goodness of fit measure; 0 means standard reduced Hi2, 1 means island-
weighted Hi2; after being optimized, S/N values is also saved)
Hi2 (tip: 0):
64.581 (S/N=151)

(FREE LINE!)

(An example of problem definition 2: up to 200 problems can be combined in one
MTP file in similar manner by single empty line dividing two problems)
Spectrum characteristics-2:
1
PM1V123.SPC
425.390 100.00 1.151 0.000
Domains - types, parameters, errors, switches, group number:
4
1 2 iso 0.2 1 1 1 1 0.25
2 2 mem 0.5 1 1 1 1 0.25
3 2 mes -1 0 0 0 0.2 0.2 1 1 1 0 1
4 2 lle 0.5 1 1 1 1 1
1 2 iso do not need to be defined
2 2 mem do not need to be defined
3 2 mes do not need to be defined
4 2 lle do not need to be defined
1 2 iso T T T T T T
2 2 mem T T T T T T
3 2 mes F F F F T T T T T T T
4 2 lle T T T T T F
2
Hi2 (tip: 0):
3.963 (S/N=20)

End of Block B (end of MTP file)
```

2.2 Output - MTP file format

The main format of data returned by EPRSIM C package is again MTP file format
with the »*name1.mtp*« if the original MTP filename was »*name.mtp*«.

The block A remains the same as is in input MTP file, parameters in block B are
replaced by optimized parameters for each problem.

Note, that the number of results is the number of problems multiplied by the number
of copies. Only the best fit from a single run of a problem is written in MTP file. To
find more than just a best fit (for example best 20 solutions found in a single run,
check POP subdirectory for POP files).

2.3 Output – _POP subdirectory and POP file format

The main data returned by EPRSIM C package further used in GHOST construction
and solution condensation is included in POP files.

In the directory where MTP files are created, EPRSIM BBW creates subdirectory for any problem defined in MTP file with the directory name equals spectral filename with »_POP« added to the end of the spectral filename.

Example: In the case of the previously described MTP file, the BBW would make 2 subdirectories with the names »*PM2V137_POP*« and »*PM1V123_POP*«.

Each subdirectory includes the following files:
- POP files with the information about the best solutions found in each run (separately in each POP file for each run) and
- TXT files with basic HEO parameters used.

The basic format of the POP file is the following:
- each line represents one solution found in HEO,
- solutions are sorted according to the quality of fit (first solutions are the best, last solutions are the worst)
- the data format in each line consist of:
  Hi2, number of components Nd, type of component 1, parameters of component 1, type of component 2, parameters of component 2, etc. up to type of component Nd, parameters of component Nd.

The POP file is used to construct GHOSTs and condense the solutions with the GHOSTmaker program.

In addition to POP files, TXT files are used to report the basic properties of the HEO of each run. The structure is the following:

```
#epr_parameters =28
#pop_size = 400
#generations = 100
#best =        15.44
Number of Simplex evaluations = 84732
Number of GA evaluations = 31369
Total number of evaluations = 116101
Sharing used FALSE
Shaking parameter =         0.50
New elite used TRUE
Selection: Tournament
Density Type: 3
```

2.4 Additional files

EPRSIM BBW reports errors (exceptions) that occur during evaluation in the form of different TXT files in the directory of MTP files.

Exceptions occurs at all levels especially because the HEO algorithm tries to jump to any possible part of the phase space and some of those parts simply do not make sense in spectral lineshape calculation.

Exceptions are handled at almost any possible level, from local modules, spectral simulation modules, computation threads and application. Therefore the report files

have different names. These files are for developing purpose only and are not interesting for end-users therefore can be deleted.

If exceptions occur regularly for some problem, the users can send the MTP files together with the exception files and the description o the problem to the authors which will tries to improve the program.