Package name: EPRSIM C – technical information

Program name: EPRSIM C library

OS environment: MS Windows (32 bit)

Purpose:

- providing all the common modules (handling files, simulation of spectra in different models and optimization algorithms) to all the programs

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1 Modules for handling files

There are several modules handling reading and writing spectral, MTP and POP files.

The structure of MTP and POP files are described in the previous chapter.

Handling of spectral files involves the following file format:

- SPC (older Bruker format)
- DTA (new Bruker format – via EPR convert program)
- ASC, DAT, ... ASCII one- or two-column text formats
- FLS, … ASCII one-column text format with text header

Here are some notes about opening spectral files (in order of appearance in the modules):

- additional Gaussian noise is added immediately after reading experimental spectral data with the amplitude as defined in MTP file,
- determination of noise – standard deviation – by fitting the outer wings (left-most and right most 100 points) of the 1024-points spectrum by two quadratic functions and sum the squares of the residuals between spectrum and quadratic fits,
- rough correction of baseline – using 1st integral – by fitting 3rd degree polynomial to the outer wings (left-most and right most 50 points) of the

1024-points 1st integral of the spectrum and subtract derivative of this polynomial baseline from the original spectrum,
- rough correction of the centre-field position – by aligning the maximum of the first integral of the simulated spectrum to the maximum of the first integral of the experimental spectrum,

Fine correction of the amplitude (normalization), centre-field and baseline are done together with spectral simulations in simulation module to adapt also to long wings of the spectra, high noise amplitudes.

2 Module for spectral simulation

The spectral simulation module includes 9 simulation models, 6 of them can be used routinely, 3 of them are for developing purpose. The models (with the 3-letter abbreviations) are:

1st model: isotropic tumbling = ISO
2nd model: anisotropic tumbling with full averaging over long axes = MEM
3rd model: isotropic spin-exchange label-label = LLE
4th model: isotropic spin-exchange label-broadening agent = LBE
5th model: anisotropic tumbling with partial averaging of all rotations = MES
9th model: spin trap simulations = TRP

Models 6 to 8 are used for developing purposes only.

Below are the model descriptions, containing model parameters, notation used in EPRSIM WIZ, units, definition intervals and parameters' normal-use switches (since some of them are implemented as constants).

General implementation notes (in the order of appearance in the algorithm):
- weighting of the spectral components is done according to double integrals (spectral intensities) is done after calculation
- linear baseline correction is done together with the amplitude normalization after weighting and composing of the spectral components
- goodness of fit is calculated after normalization and baseline correction according to the c2 type (defined in block B of MTP file) – β=0 for standard χ^2 and β=1 for first order island-weighted χ^2

$$\chi^2_{(\beta)} = \frac{1}{N}\sum_{island}\left((\lambda_{island})^{\beta} \sum_{i=1}^{\lambda_{island}} \frac{(y_{\exp} - y_{sim})^2}{\sigma^2} \right)$$

2.1 1st model = ISO: isotropic tumbling

Name of the parameter	Notation	Unit	Definition interval	Switch
proportion of Lorentzian/Gaussian mixture	L_w		0..1	T
isotropic rotational correlation time	τ_c	ns	0.02 .. 3	T
additional broadening constant	W	G	0.1 .. 4	T

polarity correction p_A	p_A		0.8 .. 1.2	T
polarity correction p_g	p_g		0.9996 .. 1.0002	T
weight	D		0 .. 1	T

Physical background and implementation notes:

- Fast motion approximation determines part of the linewidth,
- W is added to the linewidth of all lines directly

$$\frac{1}{T_2} = A\left(\tau_c, \underline{A}, \underline{g}\right) + B\left(\tau_c, \underline{A}, \underline{g}\right) M + C\left(\tau_c, \underline{A}, \underline{g}\right) M^2 + W$$

- Mixture of Lorentzian/Gaussian lineshape is calculated at the resonant line positions; L_W=0 for pure Gaussian line
- Polarity correction factor are used to correct the scalar of the tensors (trace-scalar correction)
- Hyperfine structure is added for C^{13} with the abundance determined in the MTP file (section "Tensors:")

2.2 2nd model = MEM: anisotropic tumbling with full averaging over long axes

Name of the parameter	Notation	Unit	Definition interval	Switch
order parameter S_{zz}	S		0..1	T
isotropic rotational correlation time	τ_c	ns	0.02 .. 3	T
additional broadening constant	W	G	0.1 .. 4	T
Polarity correction p_A	p_A		0.8 .. 1.2	T
Polarity correction p_g	p_g		0.9996 .. 1.0002	T
Weight	D		0 .. 1	T

Physical background and implementation notes:

- Fast motion approximation determines part of the linewidth,
- W is added to the linewidth of all lines directly (see model 1)
- Polarity correction factor are used to correct all the tensor components by the same amount (trace-scalar correction)
- S_{zz} order parameter is used to determine partial averaging of the tensor component due to wobbling of the long molecular axes
- Complete averaging is used for motions around the long axes
- Stick spectrum is generated by the numerical computation with the $\pi/2$ interval divided into 2000 steps by taking into account also transition probability correction factors up to second order
- Second order correction to stick spectrum is made near singularities by analytical expansions
- Renormalization is done to stick spectrum after all corrections
- Convolution of lorentzian derivative and stick spectrum is done up to maximal ten linewidths from each point

2.3 3rd model = LLE: isotropic spin-exchange label-label

Name of the parameter	Notation	Unit	Definition interval	Switch
isotropic rotational correlation time	τ_c	ns	0.02 .. 3	T
additional broadening const. (not exchange)	W	G	0.1 .. 4	T
Spin exchange rate	W_{ex}	G	0.1 .. 10	T
polarity correction p_A	p_A		0.8 .. 1.2	T
polarity correction p_g	p_g		0.9996 .. 1.0002	T
weight	d		0 .. 1	T

Physical background and implementation notes:

- Fast motion approximation determines part of the linewidth,
- W is added to the linewidth of all lines directly (see model 1)
- Spin exchange rate Wex is used in Bloch equation to determine lineshapes for spin-spin interacting system with the use of complex magnetization G

$$\left(\frac{1}{T_2\left(M_1\right)}+i\left(B-B_{M_1}\right)\right)\mathcal{G}_{M_1}-\sum_{M_1\neq M_2}W_{M_1M_2}\left(\mathcal{G}_{M_2}-\mathcal{G}_{M_1}\right)=-iB_1\mathcal{M}_0$$

- Polarity correction factor are used to correct all the tensor components by the same amount (trace-scalar correction)

2.4 4th model = LBE: isotropic spin-exchange label-broadening agent

Name of the parameter	Notation	Unit	Definition interval	Switch
isotropic rotational correlation time	τ_c	ns	0.02 .. 3	T
intrinsic linewidth of broadening agent	W_{Br}	G	100 .. 3000	T
concentration of broadening agent	cBr	mmol/l	100 .. 10000	T
polarity correction p_A	p_A		0.8 .. 1.2	T
polarity correction p_g	p_g		0.9996 .. 1.0002	T
weight	D		0 .. 1	T

Physical background and implementation notes – see 3rd model

2.5 5th model = MES: anisotropic tumbling with partial averaging of all rotations

Name of the parameter	Notation	Unit	Definition interval	Switch
Geometrical parameter 1	g_1		0 ..	F
Geometrical parameter 2	g_2			F
Nitroxide rotation angle 1	th	rad	0 .. π/2	F
Nitroxide rotation angle 2	fi	rad	0 .. π/2	F
main cone angle	th_0	rad	0 .. π/2	T
additional angle (locked)	psi	rad	0 .. π/2	F
asymmetry angle	fi0	rad	0 .. π/2	T
isotropic rotational correlation time	τ_c	ns	0.02 .. 3	T
additional broadening constant	W	G	0.1 .. 4	T
polarity correction p_A	p_A		0.8 .. 1.2	T
proticity prot	prot		-0.07 .. 0.07	T

weight	d		0 .. 1	T

Physical background and implementation notes:

- Polarity correction factor pA used as a scalar to correct all the A tensor components
- Proticity correction factor prot used in the following way together with g_{fe} (free electron g), p_A and empirical constants:

  $g_{xx}:=g_{xx}+(g_{xx}-g_{fe})*(-0.77*(p_A-1)-prot)$
  $g_{yy}:=g_{yy}+(g_{yy}-g_{fe})*(-0.06*(p_A-1))$
  $g_{zz}:=g_{zz}+(g_{zz}-g_{fe})*(-0.12*(p_A-1))$
- Nitroxide rotation angles 1 and 2 are used to get proper orientation of nitroxide coordinate system relative to molecular axes (axes of fast motion)
- Spectral lineshape is calculated using fast motion approximation by convolution of Lorentzian lineshape (linewidth defined in motional narrowing approximation using single effective rotational correlation time τ_c) with distribution of resonant lines (stick spectrum) which is calculated using partial averaging of the magnetic tensors' components and appropriate geometry of orientational distribution
- If effective rotation correlation time τ_c is allowed to exceed spectroscopy time window (t_{win}=3 ns), the linewidths t[j] are corrected empirically based on linewidths tt[j] at t_{win}

  $t[j]:=tt[j]-(tt[j]-t[j])*Exp(-(\tau_c-t_{win}/3)/t_{win})$
- The transformations between coordinate systems used in the algorithm bases on the following angles:
  - membrane-normal orientation dependence {Θ, Φ} and
  - orientation dependence of fastly changing rotational conformations defined with the Euler angles {ψ, ϑ, φ}

  Note that in the software "text-like" notation is used:
  - {psi, th, fi} for {ψ, ϑ, φ}
  - {TH, FI} for {Θ, Φ}

  Maximal wobble angles are denoted by the bottom-right index "0".
- Hamiltonian applied was:

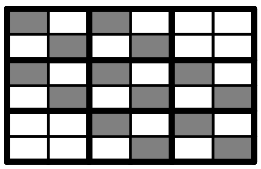
$$\hat{H} = \mu_B B\, g^{eff}\left(\vec{\Omega}\right)\hat{S}_z + \hat{\vec{I}}\; A^{eff}\left(\vec{\Omega}\right)\hat{\vec{S}}$$

  where partial averaging is taken into account with effective expressions of g and A tensor components but magnetic field orientation dependence remains explicit in vector $\vec{\Omega} = \{\Theta, \Phi\}$
- The most important averages of trigonometric functions of th0 and fi0 involves the following expressions:

$$\overline{\cos(\vartheta)^2} = \tfrac{1}{3}\left(\cos^2(\vartheta_0) + \cos(\vartheta_0) + 1\right)$$
$$\overline{\sin(\varphi)^2} = \frac{\varphi_0 - \tfrac{1}{2}\sin(2\varphi_0)}{2\varphi_0} = \frac{1}{2}\left(1 - \frac{\sin(2\varphi_0)}{2\varphi_0}\right)$$
$$\overline{\sin(\psi)^2} = \frac{\psi_0 - \tfrac{1}{2}\sin(2\psi_0)}{2\psi_0} = \frac{1}{2}\left(1 - \frac{\sin(2\psi_0)}{2\psi_0}\right)$$
$$\overline{\sin(2\vartheta)} = \tfrac{2}{3}\left(\cos(\vartheta_0) + 1\right)\sin(\vartheta_0)$$

$$\overline{\cos(\psi)} = \frac{\sin(\psi_0)}{\psi_0}$$

- Hamiltonian matrix is solved in "S_z *(I_z, I_+, I_-) terms only"* approximation with relative accuracy 0.01%, absolute accuracy 0.01 mT (including diagonals of the super-block-diagonal and sub-block diagonal)



- Resonant line position are calculated from

$$\Delta E_{M_I} = h\nu \quad \rightarrow \quad B = \frac{h\nu - M_I \sqrt{\left(A_{zz}^{eff}(\Theta_i,\Phi_i)\right)^2 + 2\left|A_{xzyz}^{eff}(\Theta_i,\Phi_i)\right|^2}}{\mu_B \; g^{eff}(\Theta_i,\Phi_i)}$$

with additional expressions

$$A_{zz}^{eff}(\Theta_i,\Phi_i) = \left(\tilde{A}_{xx}^{avg}\cos^2(\Phi_i)\sin^2(\Theta_i) + \tilde{A}_{yy}^{avg}\sin^2(\Phi_i)\sin^2(\Theta_i) + \tilde{A}_{zz}^{avg}\cos^2(\Theta_i)\right) \quad \left(g^{eff}(\Theta_i,\Phi_i)\right)^2$$

$$A_{xzyz}^{eff}(\Theta_i,\Phi_i) = \left[\frac{1}{2}\left(\tfrac{1}{2}\left(\tilde{A}_{xx}^{avg}\cos^2(\Phi_i) + \tilde{A}_{yy}^{avg}\sin^2(\Phi_i) - \tilde{A}_{zz}^{avg}\right)\sin(2\Theta_i)\right)\right.$$
$$\left. + \frac{i}{2}\left(\tfrac{1}{2}\left(\tilde{A}_{xx}^{avg} - \tilde{A}_{yy}^{avg}\right)\sin(2\Phi_i)\sin(\Theta_i) + \tilde{A}_{xz}^{avg}\sin(\Phi_i)\cos(\Theta_i)\right)\right] \quad \left(g^{eff}(\Theta_i,\Phi_i)\right)^2$$

$$\left(g^{eff}(\Theta_i,\Phi_i)\right)^2 = \tilde{G}_{xx}^{avg}\cos^2(\Phi_i)\sin^2(\Theta_i) + \tilde{G}_{yy}^{avg}\sin^2(\Phi_i)\sin^2(\Theta_i) + \tilde{G}_{zz}^{avg}\cos^2(\Theta_i)$$

and

$$\begin{aligned}
\tilde{G}_{xx}^{avg} &= g_{xx}^2\left(\overline{\cos^2(\varphi)}\,\overline{\cos^2(\vartheta)}\,\overline{\cos^2(\psi)} + \overline{\sin^2(\varphi)}\,\overline{\sin^2(\psi)}\right) \\
&\quad + g_{yy}^2\left(\overline{\sin^2(\varphi)}\,\overline{\cos^2(\vartheta)}\,\overline{\cos^2(\psi)} + \overline{\cos^2(\varphi)}\,\overline{\sin^2(\psi)}\right) \\
&\quad + g_{zz}^2\,\overline{\sin^2(\vartheta)}\,\overline{\cos^2(\psi)} \\
\tilde{G}_{yy}^{avg} &= g_{xx}^2\left(\overline{\cos^2(\varphi)}\,\overline{\cos^2(\vartheta)}\,\overline{\sin^2(\psi)} + \overline{\sin^2(\varphi)}\,\overline{\cos^2(\psi)}\right) \\
&\quad + g_{yy}^2\left(\overline{\sin^2(\varphi)}\,\overline{\cos^2(\vartheta)}\,\overline{\sin^2(\psi)} + \overline{\cos^2(\varphi)}\,\overline{\cos^2(\psi)}\right) \\
&\quad + g_{zz}^2\,\overline{\sin^2(\vartheta)}\,\overline{\sin^2(\psi)} \\
\tilde{G}_{zz}^{avg} &= g_{xx}^2\,\overline{\cos^2(\varphi)}\,\overline{\sin^2(\vartheta)} + g_{yy}^2\,\overline{\sin^2(\varphi)}\,\overline{\sin^2(\vartheta)} + g_{zz}^2\,\overline{\cos^2(\vartheta)}
\end{aligned}$$

$$\widetilde{G}_{xz}^{avg} = 0 \qquad \widetilde{G}_{xy}^{avg} = 0 \qquad \widetilde{G}_{yz}^{avg} = 0$$

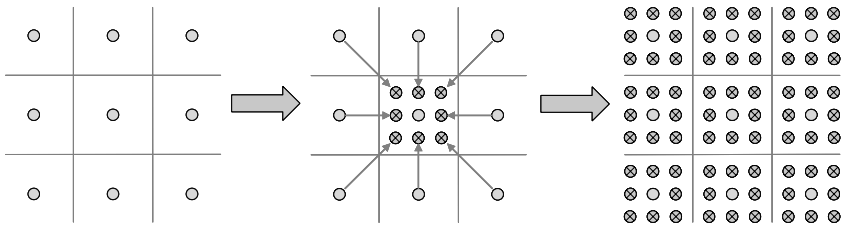
$$\widetilde{A}_{xx}^{avg} = \frac{A_{xx}}{g_{xx}^2}\left(\overline{\cos^2(\varphi)}\,\overline{\cos^2(\vartheta)}\,\overline{\cos^2(\psi)} + \overline{\sin^2(\varphi)}\,\overline{\sin^2(\psi)}\right) + \frac{A_{yy}}{g_{yy}^2}\left(\overline{\sin^2(\varphi)}\,\overline{\cos^2(\vartheta)}\,\overline{\cos^2(\psi)} + \overline{\cos^2(\varphi)}\,\overline{\sin^2(\psi)}\right) + \frac{A_{zz}}{g_{zz}^2}\,\overline{\sin^2(\vartheta)}\,\overline{\cos^2(\psi)}$$

$$\widetilde{A}_{yy}^{avg} = \frac{A_{xx}}{g_{xx}^2}\left(\overline{\cos^2(\varphi)}\,\overline{\cos^2(\vartheta)}\,\overline{\sin^2(\psi)} + \overline{\sin^2(\varphi)}\,\overline{\cos^2(\psi)}\right) + \frac{A_{yy}}{g_{yy}^2}\left(\overline{\sin^2(\varphi)}\,\overline{\cos^2(\vartheta)}\,\overline{\sin^2(\psi)} + \overline{\cos^2(\varphi)}\,\overline{\cos^2(\psi)}\right) + \frac{A_{zz}}{g_{zz}^2}\,\overline{\sin^2(\vartheta)}\,\overline{\sin^2(\psi)}$$

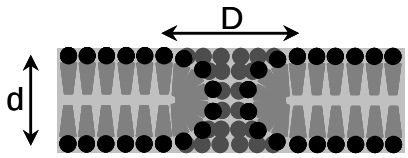
$$\widetilde{A}_{zz}^{avg} = \frac{A_{xx}}{g_{xx}^2}\,\overline{\cos^2(\varphi)}\,\overline{\sin^2(\vartheta)} + \frac{A_{yy}}{g_{yy}^2}\,\overline{\sin^2(\varphi)}\,\overline{\sin^2(\vartheta)} + \frac{A_{zz}}{g_{zz}^2}\,\overline{\cos^2(\vartheta)}$$

$$\widetilde{A}_{xz}^{avg} = 0 \qquad \widetilde{A}_{xy}^{avg} = 0 \qquad \widetilde{A}_{yz}^{avg} = 0$$

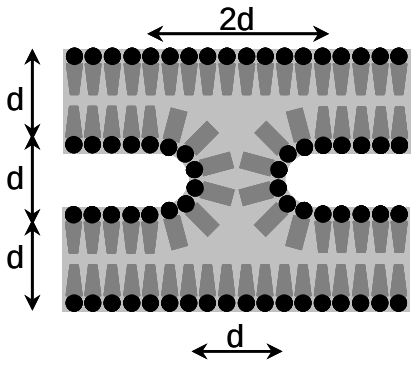
- Stick spectrum is calculated based on the 2D-extrapolation of the master grid over TH and FI (orientation relative to magnetic field) where the numbers of master steps in TH and FI dimensions correspond to the rounded quotient between the maximal resonant field change for particular π/2 rotation and resolution which is 0.6 G; master grid is extrapolated to increase resolution for 1 order of magnitude by saving 99% of grid calculation time



- Geometrical parameter 1 (g_1) is used to define geometry of the orientational distribution relative to magnetic field:
  - g_1=-1 is used to define isotropic distribution
  - g_1=0 is used to define planar distribution (perpendicular to magnetic field)
  - g_1=-2 is used to define cylindrical distribution (symmetry axis parallel to magnetic field)
  - $0<g_1<1$ is used to define pore distribution where g_1 represents the ratio between the bilayer thickness d and the pore outer diameter D:



if g_1=1/2 it can represent also neck distribution:



- Renormalization is done to stick spectrum after all corrections
- Convolution of Lorentzian derivative and stick spectrum is done up to maximal ten linewidths from each point

2.6 9th model = TRP: spin trap simulations

Name of the parameter	Notation	Unit	Definition interval	Switch
proportion of Lorentzian/Gaussian mixture	L_w		0..1	T
additional broadening constant	W	G	0.1 .. 4	T
polarity correction p_g	p_g		0.9996 .. 1.0002	T
spin of nucleus 1	S_1		Half integer: 0 .. 5	F
number of nucleus 1	N_1		Integer: 0 .. 10	F
hyperfine coupling with nucleus 1	a_1	G	0 .. 50	T
spin of nucleus 2	S_2		Half integer: 0 .. 5	F
number of nucleus 2	N_2		Integer: 0 .. 10	F
hyperfine coupling with nucleus 2	a_2	G	0 .. 50	T
spin of nucleus 3	S_3		Half integer: 0 .. 5	F
number of nucleus 3	N_3		Integer: 0 .. 10	F
hyperfine coupling with nucleus 3	a_3	G	0 .. 50	T
spin of nucleus 4	S_4		Half integer: 0 .. 5	F
number of nucleus 4	N_4		Integer: 0 .. 10	F
hyperfine coupling with nucleus 4	a_4	G	0 .. 50	T
spin of nucleus 5	S_5		Half integer: 0 .. 5	F
number of nucleus 5	N_5		Integer: 0 .. 10	F
hyperfine coupling with nucleus 5	a_5	G	0 .. 50	T
weight	d		0 .. 1	T

Physical background and implementation notes:

- Up to 5 different nuclei can be coupled to one radical (component)
- For each group (type of nuclei) multiplet positions and amplitude of lines is calculated using binomial coefficients and hyperfine coupling of the particular nuclei

- Convolution with mixture Lorentzian/Gaussian lineshape is implemented; L_w=0 for pure Gaussian line

3 Modules for parameters' optimization

The EPRSIM library contains two routines for optimization of spectral parameters: Downhill Simplex (DSO) and Hybrid Evolutionary optimization (HEO, hybridized Genetic algorithm). Both algorithms are optimized for the application of optimization of EPR spectral parameters.

DSO is used as a fast local optimization method (fine tuner) and needs good starting point to converge effectively. DSO can be used also within EPRSIM WIZ to fine tune current parameters.

HEO is used as an automatic global optimization method and need no starting conditions. HEO is combination of genetic algorithm and DSO, which is called as an operator of local mutation. HEO cannot be used within EPRSIM WIZ, but is used as a default optimization method for any problem in EPRSIM BBW, especially when searching for more reliable characterization, which requires global scan.

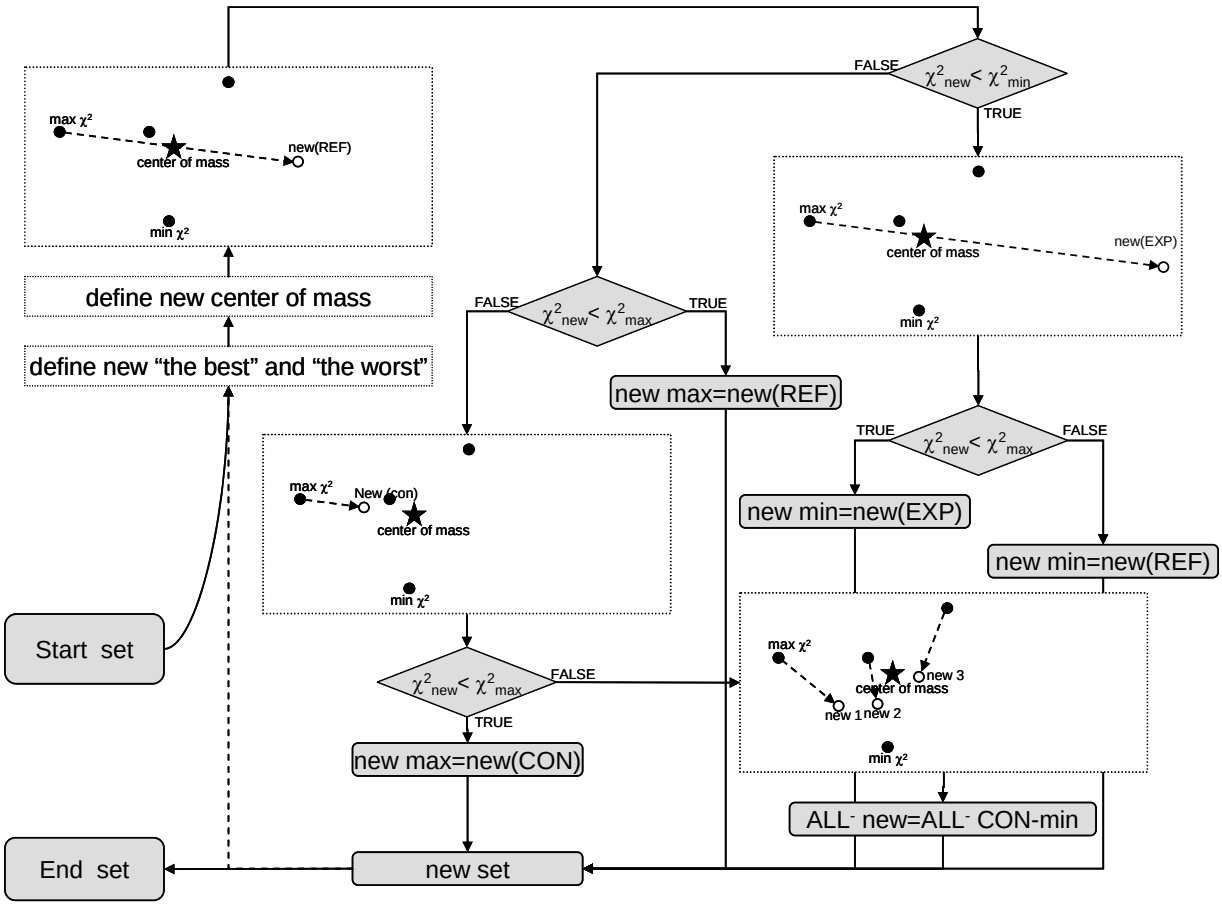
General implementation note:
Particular spectral parameter is optimized only if its switch is "true".

3.1 Simplex downhill optimization (DSO)

DSO bases on linear transformations of a population of N_p+1 points (each point is a set or vector of all spectral parameters $\{p_i\}$), where N_p is the number of optimizing parameters.

Starting population is usually created from an input vector $\{p_i,0\}$ by modifying the i^{th} parameter of the i^{th} point of the population for a small step δ_i. The size of this step is defined in MTP file in section "Grids:".

Main loop consist of four linear transformations of the worst or all point(s) relative to the center of mass (originally calculated without the worst point; see Figure below):
- reflection of the worst point across center of mass,
- reflection of the worst point across center of mass and expansion away,
- contraction of the worst point in direction of the center of mass, and
- contraction of all-except the best point toward the best point.



The stop criteria for DSO used in EPRSIM C is either:

- change of χ^2 between two successful steps which should be lower than squared noise level or
- maximal number of steps achieved where maximal number of steps is defined as a product of number of spectral (optimized parameters) and maximal number of steps per parameter. The later is defined in MTP file in 2nd line after "Downhill Simplex:" with the usual value of 55.

Special implementation notes:

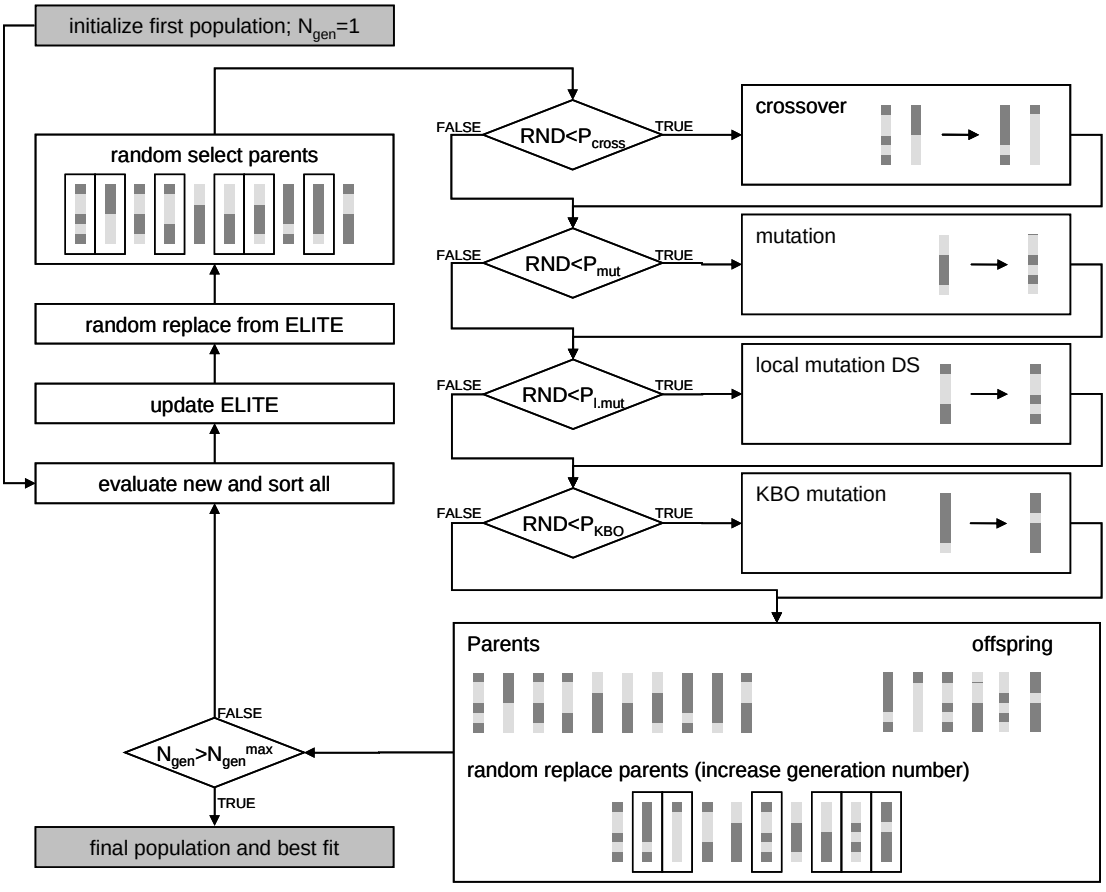
- parameters' definition intervals are defined with min and max values in MTP file ("Limits:" section)
- grids defined in MTP file (section "Grids:") are used to define first step ("simplex")
- center of mass is calculated without the worst point
- reflection involves mirroring of the calculation points over center of mass
- expansion involves 2-times expanded mirroring of the calculation points over center of mass
- minimum number of steps is 40

3.2 Hybrid evolutionary optimization (HEA = GA hybridized with DS)

Generational genetic algorithm (GA) bases on genetic-like transformations of parameters of a large population of M points, where $M >> N_p$, (each point is a set or vector of spectral parameters $\{p_i\}$), where N_p is the number of optimizing parameters. GA belongs to a family of evolutionary optimization methods; therefore it is sometimes denoted as EO. When GA is hybridized with local search operator (like SD) and knowledge-based operators, it is called Hybrid Evolutionary Optimization (HEO).

Starting population is usually created randomly within definition intervals $[p_{i,min}, p_{i,max}]$.

Main loop consist of the selection, real coding and application of genetic operators in the following scheme (see Figure below):
- fitness (χ^2) function evaluation for all new individuals
- sorting
- elitism implementation
- fitness-proportional or tournament selection
- genetic-operations application:
    - multi-point/uniform crossover
    - uniform mutation
    - local mutation (DSO)
    - knowledge-based operators
- random replacement



The stop criteria for HEO used in EPRSIM C is maximum number of generations, which is 100.

Special implementation notes:

- parameters' definition intervals are defined with min and max values in MTP file ("Limits:" section)
- grids defined in MTP file (section "Grids:") are used to define first step ("simplex")
- generation number is 50, 100, 100, 100 for up to 8, 8 - 14, 14 - 20 parameters and above, respectively
- population size is 130, 200, 280, 400 for up to 8, 8 - 14, 14 - 20 parameters and above, respectively
- number of crossover sites in multipoint crossover is 1, 1, 3 and 3 for up to 8, 8 - 14, 14 - 20 parameters and above, respectively
- other parameters (mutation probability, crossover probability, DSO probability, KBO probability, elite size) are defined in MTP file ("Hybrid Evolutionary Algorithm" section)
- elite cannot contain more than one copies of the same solution
- elite solutions replace the worst in the population every generation if the the elite solutions cannot be found in the existing population (to prevent crowding of the same solution)
- tournament selection is used to determine the pool of solution that will be transformed by genetic operators (better solutions win for selection in random pairs)
- random selection is used for selection the pair of the solutions from the pool of tournament-selected solutions
- shaking is applied within the crossover with the shaking amplitude defined from product of Gaussian-randomly deviation (amplitude 0.5) and grids (defined in MTP file in "Grids:" section)
- knowledge based operator (KBO) 1 – $\tau_{c,1}$-d_1-$\tau_{c,2}$-d_2 equilibrator – multiplies smaller τ_c by 1.3 and larger by 0.7 and subtract half of the smaller weight from the weight of the component that has larger τ_c value and add the same amount to the other one
- knowledge based operator (KBO) 2 – W_1-d_1- W_2-d_2 equilibrator – multiplies smaller W by 1.3 and larger by 0.7 and subtract half of the smaller weight from the weight of the component that has larger W value and add the same amount to the other one
- knowledge based operator (KBO) 2 – polarity sorter – remix the polarity correction factors p_g of the components in the opposite order of the sorted polarity correction factor p_A; note that polarity sorter should not be used for 5th model (MES)
- DSO is implemented as a mutation operator with probability defined in MTP file (section "Hybridization with DS during HEA")
- Resolution Auto tune adopt the grid for the (GA) mutation operator (initially defined by the grid constants from MTP file to standard deviations found by covariance matrix analysis every 10 generations
- after maximal generation number is achieved, substitution from elite is done one more, population is sorted, single DSO is used on solutions of the better part of population as defined in MTP file (section "Hybridization with DS after HEA" – possible usage and part of population should be defined)