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# CEvoS 5.0

C Evolution System

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## 1 Introduction

CEvoS – CEMoS Evolution System– is an extension of CEMoS

(Hamberg & Kohlmeier, 2023) which allows an optimization of model parameter values in respect to a given reference run. This reference run can either be another model run or a preprocessed run of field data. The package **MoViE** (Kohlmeier & Hamberg, 2023) provides a pre-processing routine for transforming field data to the structure of a model run

## (prepare tool $\rightarrow$ [data $\rightarrow$ outc] ).

The basic idea is to determine the distance of a reference run and a simulation run depending on the actual parameter set and to minimize this distance by varying the parameters. These distance is often also called cost function. The base for the calculation of the distance are all variables which are stored in both, the reference run and the simulation run. The implemented calculation of the distance is described in section 1.5.8. **CEMOS** allows the variation of all parameters defined in the file cevos.dat which must exist defined in a directory <model\_dir>/cevos. This parameters are either varied by a defined series or by random. After every calculation the resulting distance is compared to the former distance. The best parameterization is stored in bestpar.bat, the best distance in bestdist.dat and the run itself in

best.outc. For the decision which is the best distance three optimization algorithms are implemented (section 1.5.13).

If the system has been started by Start Rnd (section 1.5.13) one parameter defined in cevos.dat is varied randomly by 10% of the value at maximum. The optimization cycle will run until Stop Rnd is pressed. If the system is restarted again the optimization process will start with the last best parameterization.

**CEvoS** also allows sensitivity analyses. For this a simulation series can be started where a selected parameter is varied by a pre-determined increment in a pre-determined range. If a series has been calculated **CEvoS** stops automatically after this series. The distances to the reference run are stored.

All simulation runs are stored in <model\_dir>/cevos. The last run is always named result0.outc. If it is the best run it is copied to best.outc. In case of a random start only the last run is kept to avoid storage overflow.

WARNING: Other files than files used by CEvoS in the directory cevos are deleted during the run of CEvoS. Do not store any information in the directory cevos!!

The simulation of a model is similar to the simulation within the **CEMTK** shell. All parameter changes are read from the cemos.par resp def-files. Alternatively can the simulation be started using a cin-file. In both cases the values of the parameters defined in cevos.cev are overruled by the values defined in cevos.cev.

## 1.1 The idea of parameter adaption

The optimization of parameter can be summarized as follows.

- 1. Defining the parameters to be optimized (see 1.3)
- 2. Defining a target; a reference run. This reference run can either be another model run or a pre-processed run of field data (see 3)
- 3. Determination a cost function or distance function (see 1.5.8)
- 4. Determination an optimization method and escape criteria (see 1.5.13)

## 1.2 Requirements and Installation of CEvoS

**CEvoS** is part of **Tiger Graphics TigerPack** and an addendum of **CEMoS** and **Mo ViE**. For installtion see **CEMoS** manual. After the installation of **CEMoS/CEMTK** and **MoViE**, **CEvoS** is available and ready for use. Before starting, the parameters to be varied have to be defined.

## 1.3 Defining a parameter set for the optimization – the file cevos.cev

Before starting **CEvoS** the directory <model\_dir>/cevos must exist containing at least on file with the extension cev. This file specifies the model parameters which should be trained. If the file is named cevos.cev it is read by default. Files with other names can be selected by [CEV Files]. There are to alternatives for the syntax of this file:

1. def-file syntax Parameters are set similar to the settings in the def files, f.e.

a=3.0; /\* Parameter a \*/ b=2.5; /\* Parameter b \*/

The comments are evaluated as description. In this notation only the column value in the **CEvoS** window is valid. No series run is possible. In the case of an optimization run, no interval is evaluated. In the case of indexed variables the values must be given separately, f.e.:

```
a[1]=1.5; /* Parameter a[1] */
a[2]=3.5; /* Parameter a[2] */
```

2. %series syntax A range for the parameters can be given similar to the series in bat files., f.e.

a:0.1:0.5; /\* Parameter a \*/

where the first identifier is the parameter name, the second the minimum value ueand the third the maximum value. In this notation the column from contains the minimum value and to the maximum value.

If an optimization run is started the parameters are varied within the interval defined by the values in the columns from and to. If from and to are equal no limitation for the parameter variation is evaluated (exception :Positive Par is enabled 1.5.11).

If the optimization run should be started with a special initial value it can be defined in the sixth column

```
a:0.1:0.5:0.05:/* Parameter a */: 0.12;
```

In this case the simulation starts with this predefined starting value, otherwise it starts with the average of from and to. If the randomly chosen parameter exceeds the interval, the parameter is set to the predefined starting value (if existing) or to the average of from and to.

In the case of the optimization run the parameter for the increment is not evaluated (but must be set for consistency).

Two auxiliary scrips exist to get cev-files from def-file resp. to define a series file with ranges (see4).

## 1.4 Starting CEvoS

To start **CEvoS**, go to the directory where an existing and compiled **CEMoS** model (the file cemos.par) is located and give the command

cev cemos.par

The **CEvoS** windows appear (figure 1.1).

20				Tiger Graphics CE	voS		^ _ U X						
MODEL /hor	me/cora/data/Spl	ekeroog/Messofabl	aus Datenbank/FIMo				Stop Rupping Model						
Global Log	ine oor a data opr	oneroog, nicoopham_					and printing model						
Distance: 1													
Parameter Ch	anges												
1													
Optimisation	Parameters												
	Parameter	from	Value (absbest)	to	start	Meaning	undock						
	rass0P1	3.0	3.0	3.0	3.0	1/d maximum growth rate at 10 C							
	rup0P1	0.5	0.5	0.5	0.5	1/d nutrient uptake rate							
	rres0P1	0.14	0.14	0.14	0.14	1/d rest respiration							
	rlys0P1	1.0	1.0	1.0	1.0	1/d stress lysis rate							
	mortP1	0.0004	0.0004	0.0004	0.0004	1/(mg C/m3 *d) quadratic mortality							
	NphalfP1	0.2	0.2	0.2	0.2	mmol P/m3 half saturation value for phosph	ate uptake						
	NnhalfP1	2.6	2.6	2.6	2.6	mmol N/m3 half saturation value for nitroge	n uptake						
Ontimisation	Statue				l		M						
Best distance	17.896338	ctual Distance Inf	Absolute Best	Distance 17.896338	Runs 5041	Runs since last change 8 Broken ru	uns 652						
-File Control			710001410 00011			-Ru	n Control						
			- Marana fabiliana Batanbara										
Reference	e File /nome/o	cora/data/Spiekeroo	g/messprani_aus_Datenban	K/EIMO/Cevos//dat	a/Training_dm_sy		Start Rhd Stop Rhu						
CEV FI	le /home/o	cora/data/Splekeroo	g/Messpfahl_aus_Datenban	k/EIMo/cevos/cevos	s.cev								
CIN FI	le												
Distances & O	ptimization Contr	ol											
Distance: P	· Pointwise 1: w*(a)	t)-f(t))^2	ge all active	ar	Optir	nization: • exact • threshold acceptin	g 🔘 simulated annealing						
Ontimization	Parameters	-,, - • • • • • • • • • • •		<u> </u>			5						
Variation ra	te: 5.0 Bla V	arlation rate: 10.0	Max. steps 50 Max.	runs 500 Temr	p./Thres.: 1	Annealing rate: 0.9							
	Sig Dig I		mux.										
License	Options	Rename		Rese	t to Best Re	set to AbsBest Reset Tiger Graphi	cs MoVIE Exit						

Figure 1.1: CEvoS

A optimization run is started with [Start Rnd]. The parameter values are modified by random (in the given range) (see 1.5.13). The actual parametrization is displayed. The best simulation will be stored as best.outc. A single run can be stopped by Stop running model. The series is continued with the next random parameter set. The series is stopped by [Stop Rnd]. [Reset to Best] will set the parameters to the last best parameter set if exists.

#### 1.4.1 Starting CEvoS in batch mode

It is also possible to start **CEvoS** without GUI. To start **CEvoS** in batch mode without GUI, go to the directory where an existing and compiled **CEMoS** model (the file cemos.par) is located and give the command cev

In this case the evolution run is started. To interrupt the optimization, press Ctrl>-c. The optimization run can be customized by the settings in the file cevos.init (see 1.6).

## **1.5** The graphical user interface (GUI)

#### 1.5.1 Global log

Within this window all information during simulation etc. is listed.

#### 1.5.2 Parameter changes

Within this window all parameter changes of the actual simulation are listed. This includes changes from **CEMoS** fichange sttements.

#### 1.5.3 Optimization Parameters

Within this window the parameters to be optimized are listed. Depending on the settings in the file cevos.dat each line represents one parameter. The first column contains a checkbutton. The parameter can be enabled or disabled. If the parameter is disabled no variation of its value takes place. The second column contains the name of the parameter , the third its meaning as defined in the comment, the column from contains the minimum value of the parameters. The column value contains the actual value of the parameter. The column to contains the maximum value. This window can be undocked by undock. After closing the undocked window it is docked again.

#### 1.5.4 Best distance and Runs

The actual best distance, the actual absolute best distance is displayed. The number of runs, the number of runs after the last change of the best distance and the total number of broken runs (runs which could not be finished for any reason) is displayed. The best distance, the difftype and the number of runs is stored in the file best.dist (see 2.2).

#### 1.5.5 [Reference File]

A reference-file must be determined for the calculation of the distances. This reference file must have the structure of a **CEMoS** result file (see 3). The distances are calculated for all variables which are stored in the reference file and in the simulation result files. A reference file can also be made from field data. For further information see 3.

## 1.5.6 [cev File]

By default the file cevos.cev is read. Other cev-files can be selected.

## 1.5.7 [cin File]

By default no cin file is read. For more information, see **CEMoS**-manual.

#### 1.5.8 Distances

Two types of distances are available: pointwise distances and L2 distances. The pointwise distances compare the reference file and the actual simulation at every stored time step. The L2 distances make Fourier analyses of both, the reference file and the actual run and compare the spectral values. It is either a pointwise or a L2 distance active. The active distances is displayed.

The distances are not normed to a common maximum value so that the values calculated with different distance types are not comparable. Thus, if a previous distance calculation is done with a different distance type, a message is given and the simulation stops. In this case the stored best distance and best files must be deleted before restating the simulation by [Reset].

#### 1.5.9 Pointwise distances

The pointwise distance of the reference file and the simulation run is determined in two steps. First, the distance between every single stored variable is determined for the stored time window and normed by the number of time steps. Afterwards the resulting distance values for the different variables are averaged. The resulting number is the distance of the two files. The intermediate distances for the variables are stored in the file by [Calculate Distances]. Actually six pointwise distance types are available. Assuming that  $x_{\rm ki}, \ k = 1..K, i = 1..N$  are the results from a reference file x for a variable k and  $y_{\rm ki}$  the results from the simulation y, than the distances d(x,y) are calculated as follows:

1. 
$$d_1(x, y) = \frac{1}{2} \frac{1}{K} \sum_{k=1}^{K} \frac{1}{N} \sum_{i=1}^{N} w_k (x_{ki} - y_{ki})^2 \quad w_k = \frac{\max_k \overline{x_k}}{\overline{x_k}}$$

where  $\overline{x_k}$  is the time average of variable k of the reference file (Spitz *et al.*, 1998).

2. 
$$d_2(x,y) = \frac{1}{K} \sum_{k=1}^{K} \frac{1}{N} \sum_{i=1}^{N} \frac{|x_{ki} - y_{ki}|}{|x_{ki} + y_{ki}|}$$

3. 
$$d_3(\mathbf{x}, \mathbf{y}) = \frac{1}{K} \sum_{k=1}^{K} \frac{1}{N} \sum_{i=1}^{N} \frac{|\mathbf{x}_{ki} - \mathbf{y}_{ki}|}{\min(|\mathbf{x}_{ki}|, |\mathbf{y}_{ki}|)}$$

4. 
$$d_4(\mathbf{x}, \mathbf{y}) = \frac{1}{K} \sum_{k=1}^{K} \frac{1}{N} \sum_{i=1}^{N} \frac{|\mathbf{x}_{ki} - \mathbf{y}_{ki}|}{|\mathbf{x}_{ki}| + |\mathbf{y}_{ki}| - |\mathbf{x}_{ki} - \mathbf{y}_{ki}|}$$

5. 
$$d_5(x, y) = \frac{1}{K} \sum_{k=1}^{K} \frac{1}{N} \sum_{i=1}^{N} \ln |\frac{x_{ki}}{y_{ki}}|$$

6. 
$$d_6(\mathbf{x}, \mathbf{y}) = \frac{1}{K} \sum_{k=1}^{K} \frac{1}{N} \sum_{i=1}^{N} \left( \max(|\frac{\mathbf{x}_{ki}}{\mathbf{y}_{ki}}|, |\frac{\mathbf{y}_{ki}}{\mathbf{x}_{ki}}|) - 1 \right)$$

The distances are not normed to a common maximum value so that the values calculated with different distance types are not comparable. Thus, if a previous distance calculation is done with a different distance type, a message is given and the simulation stops. In this case the stored best distance and best files must be deleted before restating the simulation by [Reset].

The number of the distance is the same as in the distance file bestdist.dat.

#### 1.5.10 L2 distances

The so called L2 distances work on the spectral values of the runs. The transformation of the signal into spectral values allows the comparison of to results in a manner which exceeds the pointwise method by far. The comparison of simulation results and field measurements is a complicated task. The normal way is to plot both within one graph and to decide with human intuition the degree of correspondence. This is of course a very subjective decision because from psychology it is well known that people tend to see what they expect or like to see.

Such it is necessary to give an assistance to the human intuition for the exploitation of the characteristic differences and correspondings of the theoretical results and the "real life". This is only possible if not only single points are compared but the time series are compared at a whole. Only then f.e. phase shifts can be taken into account. The L2 distances are calculated as follows: In a first step a fast Fourier analyses of the reference file and the simulation run is made resulting in \_pk.outc file containing

the spectral values for every stored variable. This method works only successfully if the data are periodic in time and the stored time interval covers the period. The maximum number of complex Fourier coefficients k is – concerning the sampling theorem (Stearns (1984))– half the number of samples. Assuming N samples, the Fourier coefficients are given by a vector  $g := (g_0, g_1, ..., g_{2k}) \in \mathbb{R}^{2k+1}$  with  $k = \left\lfloor \frac{N}{2} \right\rfloor - 1$ . Thus the original value of a variable x at time t is given by

$$x(t) = \frac{1}{\sqrt{2\pi}}g_0 + \frac{1}{\sqrt{\pi}}\sum_{l=1}^k \left(g_{2l-1}\cos(lt) + g_{2l}\sin(lt)\right)$$

The norm of a time series x with the Fourier coefficients  $f_0,f_1,...,f_{2k}$  (which is an element of the room L2 – hence the name L2 distances) is given by

$$\|\mathbf{x}\| = \sqrt{\sum_{l=0}^{2k} f_l^2}$$

and the scalar product of two time series x and y with the Fourier coefficients  $f_0,f_1,...,f_{2k}$  resp.  $g_0,f_1,...,g_{2k}$  is given by

$$<\mathbf{x},\mathbf{y}>=f_0g_0+\sum_{l=0}^{2k}f_lg_l\cos(\gamma_l-\varphi_l)$$

with  $\gamma_l = \arctan\left(\frac{f_{2l}}{f_{2l-1}}\right)$  and  $\varphi_l = \arctan\left(\frac{g_{2l}}{g_{2l-1}}\right)$ . The following distance functions are implemented:

- 1.  $d_1(f,g) = ||f-g||/||f+g||$
- 2.  $d_2(f,g) = ||f-g||/min(||f||, ||g||)$
- 3.  $d_3(f,g) = ||f-g||/(||g|| + ||f|| ||f-g||)$
- 4.  $d_4(f,g) = 1 \langle f,g \rangle / (||f|| ||g||)$
- 5.  $d_5(f,g) = (||f|| ||g|| \langle f,g \rangle)/(||f|| ||g|| + \langle f,g \rangle)$
- 6.  $d_6(f,g) = \arccos(\langle f,g \rangle)/(||f|| ||g||))$
- 7.  $d_7(f,g) = |\ln(||f||/||g||)|$
- 8.  $d_8(f,g) = max(||f||/||g||, ||g||/||f||) 1$
- 9.  $d_9(f,g)=\lambda_1 d_6(f,g)+\lambda_2 d_7(f,g)$  ,  $\lambda_1=\lambda_2=1$

The distances  $d_1-d_3$ ,  $d_7$  and  $d_8$  focus on differences in the amplitudes, while distances  $d_4-d_6$  measure the phase shift. All distances are invariant concerning rotation and stretching, some are definite, surjective or fulfill the triangle inequality. Only  $d_9$  fulfills all these properties. Krug (1992) has shown that  $d_9$  is nearest to the human estimation.

WARNING: The preparation for the calculation of L2 distances (matrix inversion) can take a very long time after the first model run !! The inverted matrix is stored so that the following calculations are quite faster.

#### 1.5.11 Positive Par

If this option is set the parameter variations allows only non negative values.

#### 1.5.12 Change all active

If this option is set the parameter values of all active parameters are changed by random. Otherwise only one parameter value is changed by random. For every run the parameter to be changed is selected by random

#### 1.5.13 Optimization

The decision if the actual run is better than the actual best run can be done in different ways. The obvious method is to compare their distances (costs). relative to the reference file:

#### Exact method (EX)

The distance  $D_{act}$  is compared to the distance of the actual best run with distance  $D_{best}$  The criterion for accepting the actual run as new best run is given by

 $D_{act} < D_{best}$ 

To avoid that the optimization stucks in a local minimum the number of runs is bounded in two ways:

If the number of runs without finding a new best run exceeds Max. steps, the variation of parameters is increased (see 1.5.13).

If the number of runs without finding a new best run exceeds Max. runs, the system is new initialized by the values in the \*.cev file.

#### Threshold accepting (TA)

The exact method has the disadvantage that local minima of the cost function cannot be left. This can be reached if a run with a slighty worse distance is accepted:

 $D_{act} < D_{best} \cdot (1+T)$ 

where the threshold  ${\rm T}$  is a positive number less than 1. Thus, the actual run is accepted as new best run although its costs are higher than the cost of the actual best run.

To get convergence, the threshold value T will be gradually decreased after a predefined number of runs (see 1.5.13).

#### Simulated annealing (SA)

The simulated annealing optimization Morgan (2001) has its roots in metallurgy. Heat causes the atoms in a metal to become unstuck from their initial positions (a local minimum of the internal energy) and wander randomly through states of higher energy. Slow cooling gives them more chances of finding configurations with lower internal energy than the initial one.

By analogy with this physical process, each step of the SA algorithm replaces the actual best run by the actual run with a probability that depends on a global parameter T (called the temperature). T is gradually decreased during the process (annealing). The best run changes almost randomly when T is large, but increasingly "downhill" as T goes to zero. The acceptance of a run which is not absolutely the actual best one takes care that local minima can be left.

The criterion (Metropolis criterion) for accepting the actual run as new best run is given by

 $D_{act} < D_{best} - T \cdot \log(RND)$ 

where the temperature T is a positive number and RND a random number between zero and 1. To get convergence, the threshold value T will be reduced after a predefined number of runs (see 1.5.13).

#### Variation rate and big variation rate

The variation rate  ${\bf r}$  is the maximum variation for a positive parameter p during a run. The new parmeter is given by

$$p_{new} = p + r \cdot rnd \cdot p$$

where rnd is a random number between -0.5 and 0.5. If only positive values area allowed and  $p_{new}$  is negative, the value is refused. If the p = 0,  $p_{new}$  is set to a random number between 0 and 1 (resp. -0.5 and 0.5 if negative parameter values are allowed.)

If the exact optimization method is selected, the Variation rate increases to the Big variation rate if more than Max. Steps runs without improving the best parameter set are calculated. The variation is decreased after the next improvement.

#### Max. runs

The maximum number of runs without improvement until the optimization is reinitialized (EX). In this case the parameter values are reset to the values from the .cev file,

#### Max. steps

The maximum number of runs without improvement until the variation rate is increased (only EX).

The number of runs until the temperature resp. the threshold is decreased (TA,SA). If no improvement is reached for a specific temperature value, the system is reinitialized.In this case the parameter values are reset to the values from the .cev file. The temperature is set to its starting value.

#### Temperature, threshold and annealing rate

The temperature resp threshold  $\rm T$  controls the optimization according to 1.5.13 resp.1.5.13 . The annealing rate  $\rm r_a$  determines how fast the temperature resp. threshold decreases:

$$\mathrm{T}=\mathrm{r}_{\mathrm{a}}\cdot\mathrm{T}$$

#### [Start Rnd]

Starts the optimization. Beginning with the parameters shown in the value column the distance to the reference file is calculated. The next run is automatically started with a modified parameter set. The modifications amounts normally 10% of the absolute value of each parameter at maximum. If the value in the column from differs the value given in the column to it is additionally proved if the parameter lies in between this interval. If not the mean value of both boundaries is used as new parameter. If Positive Par is enabled only positive values are used. If a negative value is selected by random, the old value for the parameter is fixed for the next run. If the new distance is smaller than the previous the parameters are set to this better values. This process is repeated until [Stop Rnd] is pressed. The actual best parameter set is stored in bestpar.bat, the distance and the difftype is stored in bestdist.dat, the run itself is stored in best.outc.

If the distance value could not be upgraded for ten runs modifications of 100% of the absolute value of each parameter at maximum are allowed until the distance is upgraded. If the distance could not be improved for more than 10000 runs the system will be reinitialized with the original parameter values.

#### 1.5.14 [Stop Rnd]

Stops the optimization. The actual run will be finished.

#### 1.5.15 [Reset to Best]

Sets the parameters and the distance to the last best values if exist. Reads the distance and the counter from file.

#### 1.5.16 [Reset to AbsBest]

Sets the parameters and the distance to the absolute best values if exist. Reads the distance and the counter from file. The absolue best values and the best values differ if simulated annealing or threshold accepting is active.

#### 1.5.17 [Rename ]

All files belonging to a run can be renamed to keep it. The renamed files will be stored in the directory <model\_dir>/cevruns.

#### 1.5.18 [Reset]

Deletes all "'best"'-files (except the file bestpar.bat) in the directory cevos. After reset the files named absbest\* are moved to the directory cevos\_absbest in the model directory parallel to the directorycevos. The files get a time stamp. A reset should be done before changing the distance type (1.5.8).

#### 1.5.19 [Tiger Graphics MoViE ]

Starts the **Tiger Graphics** tool **MoViE** and opens directly the compare tool for the reference file and the last best run. For further information see Kohlmeier & Hamberg (2023).

#### 1.5.20 [Exit]

Closes the **CEvoS**-shell. The best-files are still available and can be read after restarting **CEvoS**.

#### 1.5.21 [CEV File]

A cev-file determing the parameters can be defined. By default the file cevos.cev is read. After changing the file the parameter window will be new initialized.

## 1.5.22 [CIN File]

A cin-file controlling the simulation can be defined (see section 19.7 in Hamberg & Kohlmeier (2023) for details). If [cancel] is pressed, no cin-file is evaluated.

## 1.5.23 [Reference File]

A .outc-file can be defined. This is taken as the goal for the training of the model under regard. All distances (pointwise or L2) are computed against the values held in this file (see 3). If [cancel] is pressed, no reference file is selected and the calculation of distances will not work.

## 1.5.24 [Stop Running Model]

A running simulation can be stopped. If the random process is running **CEvoS** continues with the next parameter set.

## 1.6 The file cevos.init

The file <model\_dir>/cevos.init is optional. If the file exist, the default settings are overruled. The file can contain the settings for the control of the optimization runs. It must be written in **Tcl/TK** notation. Example:

```
# cevos file with absolute path!!
# Default: set cev_file $cev_resultdir/cevos.cev
set cev_file $cev_resultdir/cevos.cev
# cin file with absolute path!!
# Default: none
# set cin_file
# Reference file with absolute path !!
# Default: none
# set cev_reference_file
#Optimization
#SA=0 exact EX
#SA=1 threshold acceptance TA
#SA=2 simulated annealing SA
set SA 0
# Variation rate of Parameters
set smallchange 0.1
#big variation of parameters (only SA=0)
set bigchange 1.0
#number of runs without change in best until variation
#is increased to bigchange (only EX)
#number of runs until temperature/threshold is decreased (only TA, SA)
set maxsteps 100
# number of runs without change until system is reinitialized
set maxruns 1000
#distance type
#12dis=0 point wise
#l2dist=1 L2-norm for Fourier series
set 12dist 0
#distances (cost function)
```

```
set difftype 1
# posval=0 all values
# posval=1 only positive parameters
set posval 1
#Initializing of des simulated annealing and threshold acceptance
#initial temperature (SA) resp. initial threshold (TA)
set T 1
#decreasing rate for T (SA ,TA)
set rate 0.9
```

## 2 Output Files

## 2.1 best.outc, best.info, best.log

The file best.outc is updated whenever a better distance is reached. It contains the results of the last best run. Additionally the files best.log and best.info are written. For details see **CEMoS** manual (Hamberg & Kohlmeier, 2023).

## 2.2 best.dist

The file best.dist is created whenever a model run is finished. The first row contains the actual best distance, the distance type. The third row contains the number of runs. The file will be deleted by [Reset]. If no values for comparison are available the file contains dummy values (9999999...).

## 2.3 best.bat and best.cin

The file best.bat is updated whenever a better distance is reached. It contains the best parameterization if form of a valid batch file. The parameters are also given in cin-file format (best.cin, see Hamberg & Kohlmeier (2023)).

## 2.4 The files absbest\*

The optimization with threshold acceptance (TA) and simulated annealing (SA) leads to best results which are not absolutely the best (this means that they have not the absolute minimum value for the distance but have been accepted according to the conditions of TA resp. SA). This is of special interest if several local minima of the cost function exist and the absolute best value and the best value are results from different local minima. Thus, for TA and SA the absolutely best results according to the conditions of EX are also stored in the files named absbest\*. The fact, that both are not the same is a hint that the optimization algorithm does not have converged up to know. After reset the files named absbest\* are moved to the directory cevos\_absbest in the model directory parallel to the directorycevos. The files get a time stamp.

## 3 Converting field data to comparable files

Normally field data are not available for the whole simulation period and are mostly not equidistant. For the comparison with **CEvoS** is strictly necessary to definition a reference file which has the same structure as the result files itself. The easiest way to do this is to create the reference file by the model itself. In the case of field data this is normally not useful. The **Tiger Graphics** tool **MoViE** Kohlmeier & Hamberg (2023) provides the possibility to convert field data to the format needed for **CEvoS**(see **MoViE**  $\rightarrow$  Prepare Tool  $\rightarrow$  **[data**  $\rightarrow$  **outc]**). The values are linearly interpolated. The startime, endtime, outdelt and cycle must be set to the values of the model for which the reference is designed. If the interval of the resultfile exceeds the field data, the values for the missing time stamps at the beginning and at the end are set to -9999.0. All values which are exactly -9999.0 will not be considered during the comparison. If the comparison should be done with L2 distances the (linear interpolated) reference file is automatically converted to spectral values.

**WARNING:** Actually it is not possible to select a \_dpk.outc file for reference!! (see MoViE  $\rightarrow$  Prepare Tool  $\rightarrow$  [data  $\rightarrow$  Fourier] ).

## 4 Auxiliary scripts

## 4.1 def2cev

The script def2cev converts **CEMoS** definition files (extension .def) into **CEvoS** parameter files (extension .cev). All lines not needed by **CEvoS** will be deleted. Thus, only the statments %real\_par and %real\_ind\_par are evaluated. Lines defining real\_ind\_par are splitted into single lines, f.e.:

```
def2cev xyz.def
converts the file xyz.def:
%real_ind_par
ampli[3]={1,2,3 }; /*Amplitude*/
phase[3]={0,0.25,0.5 }; /*Phase*/
freq[3]={1,1,1 }; /*Frequency*/
%globals
sinus[3];
%change
phase[1-3]={0,0.5,0.5 };
to xyz.cev
ampli[1]=1; /*Amplitude*/
ampli[2]=2; /*Amplitude*/
ampli[3]=3; /*Amplitude*/
phase[1]=0; /*Phase*/
phase[2]=0.25; /*Phase*/
phase[3]=0.5;
               /*Phase*/
freq[1]=1; /*Frequency*/
freq[2]=1;
          /*Frequency*/
freq[3]=1;
            /*Frequency*/
```

It is strictly recommended to manually correct the automatically converted files afterwards.

## 4.2 cev2ser

The script cev2ser converts a regular cev-file in parameter notation (see 1.3) to a cev-file in series notation. The script requires up to 3 arguments. First the filename to be converted, second the percentage for the modification of the parameter and

third (optional) the flag pos if only positive (including zero) values are allowed: The file xyz.cev is converted by

```
cev2ser xyz.cev 10 pos
to the file xyz_ser.cev:
ampli[1]:0.9:1.1;/*Amplitude*/
ampli[2]:1.8:2.2;/*Amplitude*/
ampli[3]:2.7:3.3;/*Amplitude*/
phase[1]:0:0.1;/*Phase*/
phase[2]:0.225:0.275;/*Phase*/
phase[3]:0.45:0.55;/*Phase*/
freq[1]:0.9:1.1;/*Frequency*/
freq[2]:0.9:1.1;/*Frequency*/
freq[3]:0.9:1.1;/*Frequency*/
```

The first value of a row is the lower boundary and the second the upper boundary. If the original value is zero, the range is set to [-percentage,percentage]. If pos is set, negative values are changed to zero. Original negative values are set to zero if pos is set.

## References

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