

```
1 SHADOWLibExtensions: methods definitions and parameters.
2 All the definitions are extracted from: Shadow3/ShadwoLibExtensions.py
3
4
5 Possible choice for col are:
6     1 X spatial coordinate [user's unit]
7     2 Y spatial coordinate [user's unit]
8     3 Z spatial coordinate [user's unit]
9     4 Xp direction or divergence [rads]
10    5 Yp direction or divergence [rads]
11    6 Zp direction or divergence [rads]
12    7 X component of the electromagnetic vector (s-polariz)
13    8 Y component of the electromagnetic vector (s-polariz)
14    9 Z component of the electromagnetic vector (s-polariz)
15   10 Lost ray flag
16   11 Energy [eV]
17   12 Ray index
18   13 Optical path length
19   14 Phase (s-polarization) in rad
20   15 Phase (p-polarization) in rad
21   16 X component of the electromagnetic vector (p-polariz)
22   17 Y component of the electromagnetic vector (p-polariz)
23   18 Z component of the electromagnetic vector (p-polariz)
24   19 Wavelength [A]
25   20  $R = \sqrt{X^2 + Y^2 + Z^2}$ 
26   21 angle from Y axis
27   22 the magnituse of the Electromagnetic vector
28   23  $|E|^2$  (total intensity)
29   24 total intensity for s-polarization
30   25 total intensity for p-polarization
31   26  $K = 2 \pi / \lambda [A^{-1}]$ 
32   27  $K = 2 \pi / \lambda * col4 [A^{-1}]$ 
33   28  $K = 2 \pi / \lambda * col5 [A^{-1}]$ 
34   29  $K = 2 \pi / \lambda * col6 [A^{-1}]$ 
35   30  $S0\text{-stokes} = |Es|^2 + |Ep|^2$ 
36   31  $S1\text{-stokes} = |Es|^2 - |Ep|^2$ 
37   32  $S2\text{-stokes} = 2 |Es| |Ep| \cos(\text{phase}_s - \text{phase}_p)$ 
38   33  $S3\text{-stokes} = 2 |Es| |Ep| \sin(\text{phase}_s - \text{phase}_p)$ 
39   34  $\text{Power} = \text{intensity}(\text{col } 23) * \text{energy}(\text{col } 11)$ 
40   35 Angle-X with Y:  $|\arcsin(X')|$ 
41   36 Angle-Z with Y:  $|\arcsin(Z')|$ 
42   37 Angle-X with Y:  $|\arcsin(X') - \text{mean}(\arcsin(X'))|$ 
43   38 Angle-Z with Y:  $|\arcsin(Z') - \text{mean}(\arcsin(Z'))|$ 
44
45
46 FROM CLASS BEAM:
47
48 def duplicate(self):
49     beam_copy = Beam()
50     beam_copy.rays = copy.deepcopy(self.rays)
51     return beam_copy
52
53 def rotate(self, theta1, axis=1, rad=1):
54     """
55
56     :param theta1: the rotation angle in degrees (default=0)
57     :param axis: The axis number (Shadow's column) for the rotation
58                  (i.e, 1:x (default), 2:y, 3:z)
59     :param file:
60     :param rad: set this flag when theta1 is in radiant
61     :return:
62     """
63
```

```
64 def traceCompoundOE(self,compoundOE,from_oe=1,write_start_files=0,write_end_files=0,\
65                       write_star_files=0, write_mirr_files=0):
66     """
67     traces a compound optical element
68
69     Note that when using write_*_files keyword, the files are written by python, not
70     by SHADOW (so FWRITE is not changed), with the exception of write_
71     mirr_files. In this case the code changes in the oe copy
72     FWRITE=1 (mirror files only). This affects the returned list of oe's
73     after tracing.
74
75     :param compoundOE: input object
76     :param from_oe: index of the first oe (for tracing compoundOE after an existing
77                     system) (default=1)
78     :param write_start_files: 0=No (default), 1=Yes (all), 2: only first and last ones
79     :param write_end_files:  0=No (default), 1=Yes (all), 2: only first and last ones
80     :param write_star_files: 0=No (default), 1=Yes (all), 2: only first and last ones
81     :param write_mirr_files: 0=No (default), 1=Yes (all), 2: only first and last ones
82     :return: a new compoundOE with the list of the OE objects after tracing (the info
83             of end.xx files)
84     """
85
86 def getshonecol(self,col, nolist=0):
87     """
88     Extract a column from a shadow file (eg. begin.dat) or a Shadow.Beam instance.
89     The column are numbered in the fortran convention, i.e. starting from 1.
90     It returns a numpy.array filled with the values of the chosen column.
91
92     Inputs:
93     beam      : str instance with the name of the shadow file to be loaded. OR
94                 Shadow.Beam initialized instance.
95     col       : int for the chosen columns.
96
97     Outputs:
98     numpy.array 1-D with length numpy.INT.
99
100    Error:
101        if an error occurs an ArgError is raised.
102    """
103
104 def getshcol(self,col,nolist=0):
105     """
106     Extract multiple columns from a shadow file (eg.'begin.dat') or a Shadow.Beam
107     instance.
108     The column are numbered in the fortran convention, i.e. starting from 1.
109     It returns a numpy.array filled with the values of the chosen column.
110
111     Inputs:
112     beam      : str instance with the name of the shadow file to be loaded. OR
113                 Shadow.Beam initialized instance.
114     col       : tuple or list instance of int with the number of columns chosen.
115
116     Outputs:
117     numpy.array 2-D with dimension R x numpy.INT. Where R is the total number of
118     column chosen
119
120    Error:
121        if an error occurs an ArgError is raised.
122    """
123
124
125
126
```

```

127 def histo1(self,col,xrange=None,nbins=50,nolost=0,ref=0,write=None,factor=1.0,\
128             calculate_widths=1,calculate_hew=0):
129     """
130     Calculate the histogram of a column, simply counting the rays, or weighting with
131     another column. It returns a dictionary which contains the histogram data.
132
133     :param col: int for the chosen column.
134     :param xrange: tuple or list of length 2 describing the interval of interest for
135     x,
136                 the data read from the chosen column. (default: None, thus using min
137                 and max of the array)
138     :param nbins: number of bins of the histogram.
139     :param nolost:
140         0    All rays
141         1    Only good rays
142         2    Only lost rays
143     :param ref:
144         0, None, "no", "NO" or "No":    only count the rays
145         23, "Yes", "YES" or "yes":      weight with intensity (look at col=23 |E|^2
146         total intensity)
147         other value: use that column as weight
148     :param write:
149         None (default)    don't write any file
150         file_name    write the histogram into the file 'file_name'.
151     :param factor: a scalar factor to multiply the selected column before
152     histogramming
153                     (e.g., for changing scale from cm to um then factor=1e4).
154     :param calculate_widths:
155     :return: a python dictionary with the calculated histogram. The following
156             keys are set:
157             error, col, write, nolost, nbins, xrange, factor
158             histogram, bins, histogram_sigma, bin_center, bin_left,
159             bin_right,
160             intensity, fwhm, nrays, good_rays,
161
162     Inputs:
163     beam      : str instance with the name of the shadow file to be loaded, or a
164                 Shadow.Beam initialized instance.
165     col       :
166
167     Optional keywords:
168     xrange    :
169     nbins     :
170     nolost    :
171     ref       :
172     write     :
173     factor    :
174     """
175
176 def histo2(self,col_h,col_v,nbins=25,ref=23, nbins_h=None, nbins_v=None, nolost=0,
177             xrange=None,yrange=None, calculate_widths=1):
178     """
179     performs 2d histogram to prepare data for a plotxy plot
180
181     It uses histogram2d for calculations
182
183     Note that this Shadow.Beam.histo2 was previously called Shadow.Beam.plotxy
184
185     :param col_h: the horizontal column
186     :param col_v: the vertical column
187     :param nbins: number of bins
188     :param ref   :
    
```

```

187         0, None, "no", "NO" or "No":    only count the rays
188         23, "Yes", "YES" or "yes":      weight with intensity (look at col=23
189             |E|^2 total intensity)
190         other value: use that column as weight
191     :param nbins_h: number of bins in H
192     :param nbins_v: number of bins in V
193     :param nolist: 0 or None: all rays, 1=good rays, 2=only losses
194     :param xrange: range for H
195     :param yrange: range for V
196     :param calculate_widths: 0=No, 1=calculate FWHM (default), 2=Calculate FWHM and FW
197         at 25% and 75% if Maximum
198     :return: a dictionary with all data needed for plot
199     """
200
201 FROM CLASS OE:
202
203
204 def set_empty(self,T_INCIDENCE=0,T_REFLECTION=180.0,T_SOURCE=0.0,T_IMAGE=0.0,ALPHA=0.0):
205     """
206     Defines an empty optical element (useful as an arm, e.g. to rotate reference frames)
207     By default, there is no change in the optical axis direction.
208
209     :param T_INCIDENCE: incidence angle (default=0)
210     :param T_REFLECTION: reflection angle (default=180)
211     :param T_SOURCE: distance from previous o.e. (default=0)
212     :param T_IMAGE: distance to next or (default=0)
213     :param ALPHA: mirror orientation angle (default=0)
214     :return:
215     """
216
217 def mirinfo(self, title=None):
218     """
219     mimics SHADOW mirinfo postprocessor. Returns a text array.
220     :return: a text array with the result
221     """
222
223 FROM CLASS CompoundOE:
224
225 def info(self,file=''):
226     """
227     write a summary of the real distances, focal distances and orientation angles.
228     :param file: set to a file name to dump result into
229     :return: a text array
230     """
231
232 def syspositions(self):
233     """
234     return a dictionary with the positions of the source, o.e. and images
235
236     :return: dic
237         dic["source"] numpy array (icoor) with the three coordinates of source
238         dic["source"] numpy array (n_oe,icoor) with the three coordinates of
239             optical elements for all elements
240         dic["source"] numpy array (n_oe,icoor) with the three coordinates of image
241             positions for all elements
242         dic["optical_axis_x"] numpy array with the x coordinates of the optical axis
243         dic["optical_axis_y"] numpy array with the y coordinates of the optical axis
244         dic["optical_axis_z"] numpy array with the z coordinates of the optical axis
245     """
246
247
248
249
    
```

```
250
251 def get_oe_index(self,oe_index):
252     """
253     returns the pointer to the oe with index oe_index
254     :param oe_index:
255     :return:
256     """
257
258 def duplicate(self):
259     """
260     Makes a copy of the compound optical element
261     :return:
262     """
263
264 def add_drift_space_downstream(self,dd):
265     """
266     Adds empty space to the last element of the compound oe
267     :param dd: The distance
268     :return: None
269     """
270
271 def add_drift_space_upstream(self,dd):
272     """
273     Adds empty space before the first element of the compound oe
274     :param dd: The distance
275     :return: None
276     """
277
278 def append(self,item):
279     """
280     append an instance of Shadow.OE or Shadow.CompoundOE
281     :param item: an OE or CompoundOE to append
282     :return: the CompoundOE updated with a copy of item appended
283     """
284
285 def append_lens(self,p,q,surface_shape=1,convex_to_the_beam=1,diameter=None,
286                 cylinder_angle=None, prerefl_file=None, refraction_index=1.0,\
287                 attenuation_coefficient=0.0,\ radius=500e-2,interthickness=0.001,\
288                 use_ccc=0):
289     """
290     Adds and sets a lens (two interfaces) to the compound optical element
291
292     :param p: distance source-first lens interface
293     :param q: distance last lens interface to image plane
294     :param surface_shape: 1=sphere 4=paraboloid, 5=plane (other surfaces not yet
... implemented)
295     :param convex_to_the_beam: convexity of the first interface exposed to the beam
... 0=No, 1=Yes
296
...         the second interface has opposite convexity
297     :param diameter: lens diameter. Set to None for infinite dimension
298     :param cylinder_angle: None=not cylindrical, 0=meridional 90=sagittal
299     :param prerefl_file: file name (from prerefl) to get the refraction index. If set
300         then the keywords refraction_index and attenuation_coefficient are not
... used.
301     :param refraction_index: n (real) #ignored if prerefl_file points to file.
302     :param attenuation_coefficient: mu (real); ignored if prerefl file points to file.
303     :param radius: lens radius (for pherical, or radius at the tip for paraboloid)
304     :param interthickness: lens thickness (distance between the two interfaces at the
305         center of the lenses)
306     :param use_ccc 0=set shadow using surface shape (FMIRR=1,4,5), 1=set shadow using
307         CCC coeffs (FMIRR=10)
308     :return: self
309     """
```

```

310
311 def append_crl(self,p0,q0, nlenses=30, slots_empty=0, radius=500e-2, thickness=625e-4,
312               interthickness=0.001, surface_shape=1, convex_to_the_beam=1, \
313               diameter=None, cylinder_angle=None, prerefl_file=None,\
314               refraction_index=1.0, attenuation_coefficient=0.0, use_ccc=0):
315     """
316     Builds the stack of oe for a CRL.
317
318     Notes: if nlenses=0 sets a single "lens" with flat interfaces and no change of
319            refraction index (like empty)
320
321            The refraction index should be input either by i) prerefl_index or ii)
322            refraction_index and
323            attenuation_coefficient keywords. The first one is prioritary.
324
325            slots_empty: if different from zero, adds a distance equal to
326            thickness*slots_empty to q0. The
327            intention is to simulate a lens that is off but the path should be
328            considered.
329
330
331
332     :param p0:distance source-first lens interface
333     :param q0:distance last lens interface to image plane
334     :param nlenses: number of lenses
335     :param slot_empty: number of empty slots (default=0)
336     :param radius:lens radius (for pherical, or radius at the tip for paraboloid)
337     :param thickness: lens thickness (piling thickness)
338     :param interthickness:lens thickness (distance between the two interfaces at the
339                        center of the lenses)
340     :param surface_shape:1=sphere 4=paraboloid, 5=plane (other surfaces not yet
341                        implemented)
342     :param convex_to_the_beam:convexity of the first interface exposed to the
343                        beam 0=No, 1=Yes the second interface has opposite convexity
344     :param diameter:lens diameter. Set to None for infinite dimension
345     :param cylinder_angle:None=not cylindrical, 0=meridional 90=sagittal
346     :param prerefl_file:file name (from prerefl) to get the refraction index. If set
347                        then the keywords refraction_index and attenuation_coefficient are not
348 ... used.
349
350     :param refraction_index: n (real) #ignored if prerefl_file points to file.
351     :param attenuation_coefficient:mu (real); ignored if prerefl file points to file.
352     :param use_ccc:0=set shadow using surface shape (FMIRR=1,4,5), 1=set shadow
353                        using CCC coeffs (FMIRR=10)
354
355     :return: self
356     """
357
358 def append_transfocator(self,p0,q0, nlenses=[4,8], slots_empty=0, radius=500e-2,
359                        thickness=625e-4, interthickness=0.001, surface_shape=1, \
360                        convex_to_the_beam=1, diameter=None, cylinder_angle=None, prerefl_file=None,
361 \
362                        refraction_index=1.0, attenuation_coefficient=0.0,use_ccc=0):
363     """
364     Builds the stack of oe for a TRANSFOCATOR. A transfocator is a stack of CRLs.
365     append_transfocator is therefore very similar to append_crl, but now arguments
366     are lists instead of scalar. However, if the value of a particular keyword is an
367     scalar and a list is expected, then it is automatically replicated "nslots"
368     times, where nslots=len(nlenses)
369
370     Notes: if nlenses=0 sets a single "lens" with flat interfaces and no change of
371            refraction index (like empty)
372
373            The refraction index should be input either by
374            i) prerefl_index or
    
```

```

371         ii) refraction_index and attenuation_coefficient keywords.
372         The first one is priority.
373
374         slots_empty: if different from zero, adds a distance equal to
375         thickness*slots_empty to q0. The intention is to simulate a lens that is
376         off but the path should be considered.
377
378         Note that all arrays must be "list". If you are using numpy arrays,
379         convert them: array.tolist()
380
381
382
383         :param p0 (list): distance previous continuation plane to first lens for each CRL
384         (usually [p,0,0,...])
385         :param q0 (scalar): distance last lens in each CRL to continuation plane
386         :param nlenses (list): number of lenses
387         :param slots_empty (list): number of empty slots
388         :param radius (list): lens radius (for pherical, or radius at the tip for
389         paraboloid)
390         :param thickness (list): lens thickness (piling thickness)
391         :param interthickness (list): lens thickness (distance between the two interfaces
392         at the center of the lenses)
393         :param surface_shape (list): 1=sphere 4=paraboloid, 5=plane (other surfaces not
394         yet implamented)
395         :param convex_to_the_beam (list): convexity of the first interface exposed to the
396         beam 0=No, 1=Yes
397         the second interface has opposite convexity
398         :param diameter (list): lens diameter. Set to None for infinite dimension
399         :param cylinder_angle (list): None=not cylindrical, 0=meridional 90=sagittal
400         :param prerefl_file (list): file name (from prerefl) to get the refraction index.
401
402     ... If set
403         then the keywords refraction_index and attenuation_coefficient are not
404         used.
405         :param refraction_index (list): n (real) #ignored if prerefl_file points to file.
406         :param attenuation_coefficient (list): mu (real); ignored if prerefl file points
407         to file.
408         :param use_ccc (scalar): 0=set shadow using surface shape (FMIRR=1,4,5), 1=set
409         shadow using CCC coeffs (FMIRR=10)
410         :return: self
411         """
412
413     def append_kb(self, p0, q0, grazing_angles_mrad=[3.0,3.0], separation=100.0,\
414         mirror_orientation_angle=0, focal_positions=[0,0], shape=[2,2],\
415         dimensions1=[0,0], dimensions2=[0,0], reflectivity_kind=[0,0],\
416         reflectivity_files=["", ""], surface_error_files=["", ""]):
417         """
418         Appends a KB (Kirkpatrick-Baez) system
419         First mirror is focusing in vertical plane, second mirror focusses in horizontal
420         plane.
421
422         Note that SHADOW rotates the image plane because the second mirror has mirror
423         orientation angle 90 ded
424
425         :param p0: distance from previous source plane (continuation plane) to center of
426         KB (!!!)
427         :param q0: distance from center of KB (!!!) to image plane (continuation plane)
428         :param grazing_angles_mrad: grazing angle in mrad for both mirrors. Default:
429         grazing_angles_mrad=[3.0,3.0]
430         :param separation: separation between the mirrors from center of first mirror (VFM)
431         to center of second one (HFM).
432         ()Default=100). T
433         he continuation plane is set in the middle.
434         :param mirror_orientation_angle: set the mirror orientation angle with respect to
    
```

```

430         the previous o.e. for the first mirror of the KB
431         :param focal_positions: the focal positions [p_focal,q_focal] measured from the
432             center of KB. If set to [0,0] then uses p0 and q0
433         :param shape: the shape code for the surfaces 1=spherica, 2=elliptical.
434             Default: shape=[2,2]
435         :param dimensions1: the dimensions [width,length] for the first mirror.
436             Default: [0,0] meaning infinite dimensions.
437         :param dimensions2: the dimensions [width,length] for the second mirror.
438             Default: [0,0] meaning infinite dimensions.
439         :param reflectivity_kind: flag for reflectivity: 0=ideal reflector, 1=mirror,
440             2=multilayer. Default=[0,0]
441             If reflectivity is set to mirror or multilayer,
442             the corresponding file must be entered in the
443             reflectivity_files keyword.
444         :param reflectivity_files: the reflectivity files, if needed. If mirror, the file
445             must have been created by prerefl. If multilayer,
446             the file must come from pre_mlayer.
447         :param surface_error_files: Set to file names containing the surface error mesh.
448             Default: surface_error_files=["",""] which means that no
449             surface error is considered.
450         :return: self
451         """
452
453     def append_monochromator_double_crystal(self, p0, q0, photon_energy_ev=14000,\
454         separation=0.0, dimensions1=[0,0],dimensions2=[0,0],\
455         reflectivity_file=""):
456         """
457         Appends a double crystal monochromator (with plane crystals)
458
459         :param p0: distance from previous source plane (continuation plane) to center of
460             double crystal monochromator
461         :param q0: distance from center of double crystal monochromator to image plane
462             (continuation plane)
463         :param set_photon_energy: photon energy in eV to set the monochromator
464         :param separation: separation between the crystals (Default=0). The continuation
465             plane is set in the middle.
466         :param dimensions1: the dimensions [width,length] for the first mirror.
467             Default: [0,0] meaning infinite dimensions.
468         :param dimensions2: the dimensions [width,length] for the second mirror.
469             Default: [0,0] meaning infinite dimensions.
470         :param reflectivity_files: the reflectivity files as created by bragg
471         :return: self
472         """
473
474     FROM CLASS Source:
475
476     def to_dictionary(self):
477         """
478         returns a python dictionary of the Shadow.Source instance
479         :return: a dictionary
480         """
481
482     def duplicate(self):
483         """
484         makes a copy of the source
485         :return: new instance of Shadow.Source()
486         """
487
488     #Gaussian source
489     def set_divergence_gauss(self, sigmaxp, sigmazp):
490         """
491         sets Gaussian source in divergence space
492         :param sigmaxp: SIGDIX for SHADOW

```



```
493         :param sigmazp: SIGDIZ for SHADOW
494         :return: self
495         """
496
497     def set_spatial_gauss(self, sigmax, sigmaz):
498         """
499         sets Gaussian source in real space
500         :param sigmax: SIGMAX for SHADOW.
501         :param sigmaz: SIGMAZ for SHADOW.
502         :return: self
503         """
504
505     def set_gauss(self, sigmax, sigmaz, sigmaxp, sigmazp):
506         """
507         Sets a Gaussian source in both real and divergence spaces
508         :param sigmax: SIGMAX for SHADOW.
509         :param sigmaz: SIGMAZ for SHADOW.
510         :param sigmaxp: SIGDIX for SHADOW.
511         :param sigmazp: SIGDIZ for SHADOW.
512         :return: self
513         """
514
515     def set_energy_monochromatic(self, emin):
516         """
517         Sets a single energy line for the source (monochromatic)
518         :param emin: the energy in eV
519         :return: self
520         """
521
522     def set_energy_box(self, emin, emax):
523         """
524         Sets a box energy distribution for the source (monochromatic)
525         :param emin: minimum energy in eV
526         :param emax: maximum energy in eV
527         :return: self
528         """
529
530     def set_pencil(self):
531         """
532         Sets a pencil beam (zero size, zero divergence)
533         :return:
534         """
535
536
537     def apply_gaussian_undulator(self, undulator_length_in_m=1.0, user_unit_to_m=1e2, \
538                                verbose=1, und_e0=None):
539         """
540         Convolves the already defined Gaussian source (for the electrons) with the
541         photon emission for an undulator.
542
543         :param undulator_length_in_m:
544         :param user_unit_to_m:
545         :param verbose: set to 0 for silent output
546         :param und_e0: the setting photon energy in eV, if undefined (None) reads from SHADOW
547                        PH1 variable
548         :return: self
549         """
550
551     def sourcinfo(self, title=None):
552         """
553         mimics SHADOW sourcinfo postprocessor. Returns a text array.
554         :return: a text string
555         """
```