

1 **pySCu: a new python code for analyzing remagnetizations directions by means of**
2 **Small Circle utilities.**

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25 Abstract:

26 The small circle (SC) methods are founded upon two main starting hypotheses: (i) the
27 paleomagnetic sites in question were remagnetized contemporaneously, acquiring the
28 same paleomagnetic direction. (ii) The deviation of the acquired paleomagnetic signal
29 from its original direction is only due to tilting around the bedding strike and therefore
30 the remagnetization direction must be located on a small circle (SC) whose axis is the
31 strike of bedding and contains the *in situ* paleomagnetic direction. The SC methods has
32 two applications: (1) The Small Circle Intersection (SCI) method is capable of
33 providing adequate approximations to an expected paleomagnetic direction when
34 dealing with synfolding remagnetizations. By comparing the SCI direction with that
35 predicted from an apparent polar wander path, the (re)magnetization can be dated. (2)
36 Once the remagnetization direction is known, the attitude of the beds (at each site) can
37 be restored to the moment of acquisition of the remagnetization, showing a unique
38 picture of the structure in the past (palinspastic reconstruction). Therefore, if we analyze
39 several sites (with different bedding strikes) their SCs will intersect in the
40 remagnetization direction. Some caveats are necessary under more complex tectonic
41 scenarios, in which SC-based methods can lead to erroneous interpretations. However,
42 the graphical output of the methods tries to avoid ‘black-box’ effects and can minimize
43 misleading interpretations or even help, for example, to identify local or regional
44 vertical axis rotations. In any case, the methods must be used with caution and always
45 considering the knowledge of the tectonic frame in which it is applied.

46 In this paper, some applications of the SC analysis are automatized by means of
47 a new Python code. With pySCu the SCs methods can be easily and quickly applied,

48 obtaining firstly a set of text files containing all calculated information and
49 subsequently generating a graphical output on the fly.

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51 **1. Introduction**

52

53 The paleomagnetic fold-test (Graham, 1949) is a basic tool for recognizing pre-,
54 syn- or post-folding magnetizations. However, for structural reconstructions using
55 synfolding remagnetizations (defining “synfolding” as either a magnetization acquired
56 between two different folding events -i.e. between the end of the first folding stage and
57 before the beginning of the second one, or during the development of a fold in a single
58 event-), this method cannot be used because the incremental fold-test (McCabe and
59 Elmore, 1989; McFadden, 1990; Bazhenov and Shipunov, 1991; Watson and Enkin,
60 1993; Tauxe and Watson, 1994) assumes proportional folding at the different limbs and
61 this is an assumption not necessarily met in nature (e.g. Suppe, 1983; Cairanne et al.,
62 2002; Delaunay et al., 2002; Villalaín et al., 2003).

63 To overcome the (sometimes) erroneous assumption of proportional folding and
64 to obtain the correct restoration of bedding, some authors proposed more detailed
65 analyses with non-symmetric unfolding of the different fold limbs. These efforts are
66 based on the fact that the transformation of a paleomagnetic vector from geographic to
67 stratigraphic coordinates (i.e. tilt correction) implies the rotation of the vector along a
68 small circle (SC) whose axis is the strike of the bed and the amount of rotation is the dip
69 angle. In this way, McClelland-Brown (1983) treated synfolding remagnetizations by
70 comparing different percentages of unfolding of the limbs and analyzing the path of the
71 paleomagnetic direction upon the corresponding SC. Surmont et al. (1990) observed
72 maximum clustering of the paleomagnetic directions after applying partial tilt
73 corrections at the sites (i.e. the space region showing higher concentration of
74 intersection between the SC); they considered this cluster as the remagnetization
75 direction and the discrepancy with the expected direction was attributed to vertical axis

76 rotation. A similar work was presented by Villalain et al. (1992) who calculated a local
77 remagnetization direction as the intersection of the SCs and restored each limb
78 separately.

79 An important step forward was done by Shipunov (1997) who clearly
80 established the Small Circle Intersection (SCI) as a useful method to calculate local
81 remagnetization directions. When the paleomagnetic direction corresponds with a
82 synfolding remagnetization (i.e. the magnetization was acquired after partial folding of
83 beds) and supposing only tilting of the beds around a horizontal axis (e.g. absence of
84 differential vertical axis rotation between each paleomagnetic site), the actual local
85 direction of the remagnetization must be coincident for all sites and located along each
86 SC. In other words, the small circles must show a common direction (or narrow spatial
87 distribution), corresponding to the local direction of the remagnetization (Shipunov,
88 1997).

89 More improvements for the SCI method were made by Henry et al. (2004), who
90 established the reliability of the method depending on the geological conditions (e.g. the
91 distribution of strikes of the beds), and modified the way to calculate the
92 remagnetization direction. They also provided a useful discussion about the
93 uncertainties in the calculation of the paleomagnetic direction (a weak point in
94 paleomagnetism in general, and in the SCI method, in particular).

95 Finally, Waldhör (1999) and Waldhör and Appel (2006) substantially improved
96 the SCI method as a tool to calculate remagnetization directions. They discussed widely
97 the applicability of the SCI method, focusing their work on testing it under different
98 conditions, such as the distribution of the strike of the beds and the corresponding
99 dispersion pattern of the intersections. In addition, these authors introduced the statistic
100 A, the sum of the minimum angles between any direction and each SC. The direction

101 minimizing A is assumed to be the remagnetization direction. Moreover, the distribution
102 of A values (or A/n , normalizing the A value for the number of sites n) for all directions
103 can be used as an indicator of dispersion of the SC distribution, or at least as an
104 indicator of the reliability of the remagnetization direction.

105 Following this line of logic, an important concept is the best fit direction (BFD)
106 which is the vector located along each SC that lies closest to the calculated
107 remagnetization direction. The angle between the BFD and the paleomagnetic direction
108 for each site before bedding correction (BBC) is the unfolding angle (Villalaín et al.,
109 2003) and the angle between the BFD and the paleomagnetic direction after total
110 bedding correction (ATBC) is the paleodip of the bed (i.e. the dip of the beds at the
111 moment of the acquisition of the remagnetization). This was the workflow followed by
112 Villalaín et al. (2003) who introduced the term of ‘asymmetrical solution’, consisting of
113 differential unfolding of each limb depending of the calculated paleodip. Hence, the
114 reconstruction of the beds using this method offers a unique image of the geological
115 structures at the moment of the remagnetization.

116 Since its introduction, several investigators have presented different applications
117 of the SC methods. Meijers et al. (2011) used their as a conventional fold test. Others
118 use SC analysis for reconstructing the paleo-geometry of sedimentary basins (Villalaín
119 et al., 2003; Soto et al. 2008; Soto et al., 2011; Casas et al, 2009; Torres-López et al.,
120 2016), for separating deformation generated under different tectonic phases (Smith et
121 al., 2006) or for relative dating of geological structures (Calvín et al., 2017). An
122 extended review of restoration using the SCI method (focused on intraplate basins) can
123 be found in Villalaín et al. (2016). They documented some promising results which
124 demonstrated the applicability of the SCI method in geological frameworks with
125 regional vertical axis rotations (VARs) generated after the acquisition of the

126 remagnetization. These VARs are added to the tilting recorded by the beds. In this
127 context, and starting from the knowledge of an external paleomagnetic reference
128 direction, it is possible to calculate the amount of tilting and VAR recorded by the rocks
129 (e.g. Waldhör et al., 2001; Antolín et al., 2012; Rouvier et al., 2012); however, more
130 knowledge about the behavior of the SCI method under tectonic frames affected by
131 VAR is necessary to avoid misleading interpretations. Finally, another use derived from
132 the calculation of the paleomagnetic direction is the dating of the remagnetization by
133 comparison with the Apparent Polar Wander Path (APWP) in local coordinates (e.g.
134 Henry et al., 2001; Gong et al., 2009; Torres-López et al., 2014). Needless to say that
135 the presence of younger regional tilting or VARs will complicate this task (e.g.
136 Jordanova et al., 2001).

137 In summary, the inherent uncertainty of the tectonic correction in synfolding
138 remagnetizations makes analysis using the SCI method useful for inferring
139 paleomagnetic directions. One of the main advantages of the SC methods for structural
140 reconstructions based on synfolding remagnetizations lies in the fact that it does not
141 assume proportional unfolding in each limb. Moreover, SC offers the possibility of a
142 graphical output allowing us to explore complex situations while minimizing possible
143 “black-box” effects. These are two key points, while the classical and progressive fold-
144 tests can be used to check the primary or secondary origin of the magnetization, the SC
145 methods have the potential for additional information. If the required external
146 conditions for applying the methods are fulfilled (actually, or as a working hypothesis),
147 they allow the calculation of the direction of a remagnetization, and of restoring each
148 site separately to the moment of the remagnetization event.

149 The main problem for the application of the SC methods was the absence of
150 software to do the necessary calculations in a straightforward way. Only two

151 unpublished software packages, one of them written by B. Henry (IPGP, Paris) and
152 another by M. Waldhör (UT, Tübingen) as an excel spreadsheet, have allowed
153 application of the SCI method to paleomagnetic datasets, although they do not provide
154 restoration utilities. Recently, the new version of VPD software (Ramón et al., 2017)
155 also allows application of the SCI method. Therefore, although it is certain that many
156 researchers are grateful for these programs, the absence of user-friendly, open source
157 software has precluded widespread application of the SC methods and its regular use
158 has been restricted to a few research groups (IPGP of Paris –France-, Tübingen
159 University –Germany-, Burgos and Zaragoza Universities –Spain).

160 In this paper, we present pySCu as the new Python-based software package
161 which allows easy calculation of the remagnetization direction (SCI solution) for a
162 dataset and provides the paleo-dip of each site (for bedding restoration) among other
163 parameters. In this way, we propose (and we consider it necessary) the routine use of
164 this method in magnetotectonic investigations in the same way that the classical fold
165 test has been used traditionally. The software is based on the iterative method for
166 calculating the remagnetization direction used in the previous software, especially
167 Waldhör's spreadsheet. In addition, pySCu provides an uncertainty ellipse for the SCI
168 solution on the basis of parametric bootstrapping techniques. Besides, it follows the
169 philosophy of the new PmagPy software package (Tauxe et al., 2016) with open source
170 code which can be easily modifiable for specific cases or for future improvements of the
171 method; in fact, the drawing module (pySCu_draw.py) uses code from PmagPy to avoid
172 repeating this code with the same aim.

173

174 **2. Theoretical background**

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176 2.1. Definition of parameters

177

178 Small circles (SCs) are the key to the SC methods. One SC corresponds to the
179 path followed by the paleomagnetic direction with progressive rotation around an axis
180 parallel to the bedding strike (Fig. 1a). For each site, the SC is defined by the bedding
181 strike (t , according to the right hand rule -RHR-) and the in situ magnetization (i.e. the
182 SC that contains the magnetization and whose axis is t) (Fig. 1a). Therefore, each SC
183 can be parametrized by t and its apical angle Ap (or by d , the cosine of Ap , since
184 calculations are performed on a unit sphere). Ap is the angle between the vector
185 magnetization and the strike.

186 The program works by minimizing angular distances. For this purpose, it must
187 calculate the minimum angular distance (α) between different directions (P, directions
188 susceptible of being the remagnetization direction, see next subsection) and each SC
189 (Fig. 1b). The minimum angular distance α is measured over a great circle that contains
190 P and whose strike is t (Fig. 1b).

191 Once the angular distances between P and each SC have been calculated, the
192 coordinates of the closest point to P located along the SC are calculated (for each SC).
193 This point (Q) correspond to the intersection between the SC and the great circle that
194 contains P (Fig. 1b).

195

196 2.2 The remagnetization direction (SCI method)

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198 The SCI method is based on the following assumptions. (i) The analyzed sites
199 were remagnetized contemporaneously and therefore they acquired the same
200 remagnetization direction. (ii) Assuming, that only tilting of the beds around the

201 bedding strike is responsible for the dispersion of the paleomagnetic directions from
202 their original direction, the remagnetization direction must be placed upon the SC that
203 links the paleomagnetic direction in BBC (before bedding correction) and ATBC (after
204 total bedding correction) (Fig. 1a). If these two conditions are true, then it follows that
205 all SCs should intersect in the remagnetization direction. For the method to work
206 effectively, the beds must have different strikes because otherwise all SCs would be
207 concentric with no intersection.

208 Because of the noise in data collection, intersections of SCs will be scattered,
209 and the typical dataset (Fig 2a) will show an area in which the intersections between the
210 different SCs cluster. According to Waldhör and Appel (2006), one way to calculate the
211 remagnetization direction is to try and find the direction that minimizes its angular
212 distances to the set of SCs. For this, the minimum angle between any particular
213 direction and the SCs (α_j) can be calculated (Fig. 1b); the value of A/n , which is the sum
214 of all individual angles (α_i) normalized for the number of sites can be calculated ($\frac{1}{n}\sum\alpha_j$,
215 Fig. 2b). The SCI solution will be the one with minimum A/n value (i.e. the closest
216 direction to the set of SCs; Fig. 2c). Once the SCI solution is calculated this becomes
217 the reference and the final points Q converge to the best fit direction (BFD), the closest
218 direction between each SC and the reference.

219

220 *2.2.1 Uncertainty estimation*

221

222 Estimating the uncertainty associated with the calculated remagnetization
223 direction is a complex issue. The difficulty stems from several aspects, such as the
224 homogeneity of the attitude of bedding (the greater the homogeneity the greater the
225 uncertainty along the SCs), the relationship between the remagnetization direction and

226 regional structural trend, the non-coaxial nature of the pre- and post-remagnetization
227 deformation, and/or the quality of the bedding and paleomagnetic data. Given an SCI
228 solution as in Fig. 2, the SC intersection pattern, as well as the A/n contour plot, gives a
229 qualitative approximation of the uncertainty associated with the calculated direction; the
230 uncertainty increases with the concentricity of the SCs and the eccentricity of A/n
231 contours (Fig. 3a). However, A/n cannot be used as the regular confidence zones used in
232 paleomagnetism with a quantitative statistical significance, precluding the use, for
233 example, of a comparison with the apparent polar wander path (APWP) for
234 remagnetization dating. This issue has been traditionally assessed by means of Fisher's
235 (1953) statistics on the BFDs. This approach has two main flaws: (i) the BFDs do not
236 usually follow a Fisherian distribution and (ii) these directions are artificially calculated
237 (the BFD corresponds with the direction on each SC closest to the calculated direction
238 which also invalidates a Fisherian approach using the BFDs). As a consequence of this
239 misuse, misleading confidence regions are obtained, and they tend to be elongated just
240 in the direction perpendicular to the actual uncertainty (Fig. 3b); BFDs are forced in the
241 uncertainty direction which is the same as the SC paths, and therefore they cannot show
242 dispersion in this direction. Another consequence is that, whereas the real uncertainty of
243 the solution increases with more concentric SC (magenta ellipse in Fig. 3), small
244 variations can be observed between the confidence zones of the BFDs (red circle and
245 black ellipse Fig. 3), indicating an absence of statistical significance of the latter.

246 Following an approach similar to Henry et al.'s (2004), the uncertainty of the
247 SCI solution can be estimated by means of confidence areas with statistical significance
248 if several solutions are calculated. This is possible if many pseudosamples of the input
249 data (i.e. paleomagnetic directions and bedding) are generated through a parametric
250 bootstrap (Fisher et al., 1987; Watson and Enkin, 1993; Tauxe and Watson, 1994).

251 Combining pairs of paleomagnetic directions and bedding, in each pseudosample, new
252 bootstrapped-SCs can be defined and used to calculate new SCI solutions. If a large
253 number of SCI solutions are calculated (e.g. more than 100), the confidence zone can be
254 calculated. In agreement with the results obtained in the previous examples (Fig. 3), the
255 dispersion of the 500 SCI solutions follows an elliptical distribution; therefore, and
256 following the work of Tauxe et al. (1991), Kent (1982) statistic is used to calculate the
257 95 % confidence ellipse.

258 The pseudosamples generated by parametric bootstrap will follow the same
259 Fisherian distribution as the input data (by design) and share Fisher's (1953) k
260 parameter. Therefore, since either the paleomagnetic direction and the bedding have an
261 error defined by the Fisherian distribution with precision parameter k (for bedding a k
262 of 120-150 can be realistic), the propagation of this error to the SCs can be introduced
263 in the SCI solution in this way, which is exactly what this confidence region implies.

264 Even when used together with the confidence region, the SCI solution can be
265 unrealistic if some of the initial assumptions are not fulfilled. For example, if the SCI
266 method is applied to a dataset affected by differential VAR, we will obtain wrong
267 solutions even having reasonable A/n distributions and confidence zones (Fig. 4). For
268 this, in our opinion, the best way to assess the uncertainty of the calculated
269 remagnetization direction is through the confidence zone and the A/n value always
270 accompanied with the SCs (or their intersections) and A/n values distribution (Fig. 4).

271

272 2.3 The paleodip calculations

273

274 The paleodip is the dip of the bedding plane at the moment of the acquisition of
275 the remagnetization, obtained from simple calculations. (i) Once the reference is known,

276 it is possible to calculate for each paleomagnetic site the direction within their
277 corresponding SC closest to it, i.e. the BFD. (ii) The angle measured along the SC
278 between the ATBC and the BFD paleomagnetic directions corresponds with the
279 paleodip (Fig. 5).

280 The frequently encountered situation working with synfolding remagnetizations
281 is the one in which the paleodip shows an intermediate position between the BBC and
282 ATBC attitudes (Fig. 5a), caused by a progressive tilting with the same sense along
283 folding time (pre- and post-remagnetization tilting show the same dip direction).
284 However, it is also possible to obtain opposite senses of tilting of the pre- and post-
285 remagnetization stage, thus giving higher paleodips than present-day dips (Fig. 5b) or
286 even changing the sense of dip of beds (Fig. 5c). In case of working with prefolding
287 remagnetizations, the paleodip will be 0° (Fig. 5d) and for postfolding remagnetizations
288 the paleodip will coincide with the present-day dip (Fig. 5e). Real examples of these
289 cases can be found in the literature (e.g. Smith et al., 2006; García-Lasanta et al., 2017,
290 among others).

291

292 2.3.1 The uncertainty in the paleodip

293

294 Uncertainty in the paleodip comes from the uncertainties in the bedding, in the
295 paleomagnetic direction of each site and in the SCI solution. Bedding and
296 paleomagnetic directions errors act at site-scale and the paleogeometry of the structures
297 can be artificially modified. Therefore, the use of sites with large paleomagnetic
298 direction uncertainties should be avoided, and just in case they can be used as a source
299 of qualitative information. Besides, this uncertainty not only affects the magnitude of
300 the α_{95} of the paleomagnetic direction, but also the apical angle of the SC: for high

301 apical angles (90° maximum), an α_{95} of 5° will generate around 5° of paleodip
302 uncertainty; however, for low apical angles (e.g. 20°), an α_{95} of 5° will generate around
303 30° of paleodip uncertainty. Regarding uncertainties in bedding attitude, this is the same
304 as for the dip and can be neglected for the purposes of reconstruction of the structure.

305 Otherwise, the uncertainty in the SCI solution is common to all sites, hence this
306 will only affect the general attitude of the sites regarding an external reference, but will
307 not affect the relative attitude between sites. In other words, the interlimb angle will be
308 constrained, but the structures can be artificially tilted.

309

310 2.4 Considerations before using the SC methods

311

312 Some caveats must be taken into account when using the SC methods for calculating the
313 reference direction and paleodips:

314

315 - There is an intrinsic ambiguity in the calculation of the reference direction (SCI
316 solution), because it is always possible to calculate two remagnetization directions with
317 the same declination and opposite inclinations (Fig. 6). Other sources of information
318 (e.g. paleomagnetic direction in horizontal sites) will be necessary to discriminate
319 between the two.

320 - For very similar strikes of bedding, the uncertainty in the calculated remagnetization
321 direction will be high (Fig. 3b; e.g. Cairanne et al., 2002; Gong et al., 2009).

322 - Because the SCI method works with remagnetization directions, we must be sure that
323 we are working with a real remagnetization and not with an artifact, which can be
324 generated by different processes. (i) Overlapping between two paleomagnetic
325 components could be interpreted as a syn-tectonic remagnetization (Rodríguez-Pintó et

326 al., 2013). (ii) Internal deformation of sedimentary beds can rotate a primary
327 paleomagnetic components that shows the same behavior that a syn-folding
328 remagnetization (e.g. Van der Pluijm, 1987; Stamatakos and Kodama, 1991).
329 Anisotropy of the remanence measurements or sampling in different lithologies (e.g.
330 limestones and marls) and therefore with different responses to deformational
331 mechanisms can shed light to avoid these problems.

332 - The weight that each SC has in the SCI solution depends on the strike distribution
333 (Waldhör and Appel, 2006). For example, in a case with several SCs defined by similar
334 strikes and a few SCs with axes at a high angle to the others, the remagnetization
335 direction will be strongly conditioned by the latter.

336 - Generally, the SC methods are useful and reliable in contexts without complex
337 tectonic histories (i.e. similar tilt axis during the pre- and post-remagnetization stages,
338 Villalain et al., 2015). Otherwise, in complex tectonic frames it can be necessary to
339 restore the most recent deformation(s) before applying the SCs methods.

340 - In tectonic contexts with VAR postdating the remagnetization, the SCI method should
341 be used with caution but it can still provide useful constraints (see Waldhör et al., 2001;
342 Waldhör and Appel, 2006; Antolín et al., 2012; Rouvier et al., 2012). For example, it
343 can be possible to assess the presence of differential VAR recorded by the different sites
344 according to the distribution of the SCs, to calculate regional VAR if the paleomagnetic
345 reference is known, etc.

346 - It is important to differentiate in these complex tectonic frames (last two points)
347 between differential and regional VARs. The first will increase the noise in the
348 calculated remagnetization direction and in the restoration. However, homogeneous
349 VARs will preclude a correct calculation of the remagnetization direction (and
350 consequently its use for dating the remagnetization); structural relationships between

351 sites will be accurate, but the general structure can be biased with respect to an external
352 reference. In these complex tectonic frames, external markers (e.g. geological markers)
353 can help to avoid these effects. According to our experience, a large dataset can help to
354 minimize the noise in the calculation of the remagnetization direction derived from
355 anomalous strikes, uncontrolled sites with local VAR, etc.

356

357 The many caveats notwithstanding, it is worth noting that most of them are
358 common to other paleomagnetic approaches applied to unravel the deformational
359 history of the mountain belts, either working with primary or secondary remanences
360 (e.g. Pueyo et al., 2016). Therefore the SC methods do not have more limitations than
361 other techniques. In any case, it is a technique that works well in simple tectonic frames,
362 but also, combined with other methods, can help to understand complex deformational
363 histories.

364

365 **3. How to use pySCu**

366

367 The pySCu program is written in Python 2.7 and consists of two different
368 modules (each with their python file). pySCu_calc.py is the main module which does
369 the calculations and pySCu_draw.py provides the graphical output for the program. This
370 can be used either as a stand alone piece of code (downloading it from GitHub.com) or
371 as a tool inside of the paleomagnetic set of tools PmagPy (Tauxe et al., 2016).

372 Following the first option (as an individual software), just search pySCu in
373 www.GitHub.com website and download it (this also incorporates a 'readme' with the
374 instructions). The program uses some basic Python libraries as Matplotlib-1.5.3 and
375 Numpy-1.11.2 so it will not run on the standard Mac OS and Windows versions of

376 python; we recommend either the Anaconda or Canopy installations. On the other hand,
377 if you choose the PmagPy installation (which includes many other paleomagnetic tools),
378 use pySCu as the other PmagPy's tools. The user is referred to the instructions for
379 PmagPy and Anaconda or Canopy installations in the PmagPy cookbook at:
380 <https://earthref.org/PmagPy/>.

381

382 3.1. pySCu_calc.py

383

384 The input data file is a spaced delimited text file with header as shown in Table
385 1. All output data files (five as maximum) have this same format. Some communication
386 with the program is necessary and they will be introduced through a command line
387 input request.

388 The pySCu_calc.py does different calculations: the parameters that define each
389 SC, the possible intersections between each pair of SCs, the SCI solution and its
390 confidence ellipse (through the calculation of 500 SCI solutions), the A/n matrix (a grid
391 with the A/n values for all possible directions) and the paleodip for each site. These
392 calculations can be performed following three different workflows (Fig. 7) depending
393 on the user's requirements. (i) The basic step (w1, Fig. 7) is to do all calculations. (ii)
394 Sometimes it can be interesting to quickly calculate remagnetization directions (w2, Fig.
395 7) using different datasets to assess the reliability of some sites without calculating the
396 A/n matrix (this takes some minutes). (iii) Finally, it is also possible to calculate the
397 paleodips of the entire dataset using a remagnetization direction either calculated
398 previously (SCI solution) or from other sources, such as the APWP (w3, Fig. 7a).

399

400

401 3.2. pySCu_draw.py

402

403 The graphical output is mostly based on the PmagPy package (Tauxe et al.,
404 2016). After running the program, it asks about the **main.txt* output file generated with
405 *pySC_calc.py*. Then, a set of four equal area plots is generated (Fig. 8) representing the
406 SCs, the BBC, BFD and ATBC paleomagnetic directions, the contour plot of the A/n ,
407 the 500 SCI solutions and the intersections of the SCs (the last three are optional).
408 Besides, a modified version of this module is available (*pySCu_draw_labels.py*); this
409 module draws only one equal area plot with the SCs, the reference direction, the BBC,
410 BFD and ATBC paleomagnetic directions and the labels of the different sites. This is
411 meant to use with few sites, for example for showing the results coming from a single
412 fold.

413 Output plots from these modules are drawn with the matplotlib library and
414 therefore they follow the design of this library. One important question is that this
415 library allows saving the plots in different formats. The code of *pySCu_draw.py* is
416 easily modifiable to change the color, the size or the shape of the different elements as
417 well as the configuration of the contour plot (just open it with a code editor).

418

419 **4. How does pySCu work?**

420

421 4.1. The iterative approach

422

423 The main workflow proceeds through an iterative approach (Fig. 9) in order to
424 find the direction closest to the set of SCs, i.e. the SCI solution (Fig. 2). Given a starting
425 point (P_0), the program calculates, for each site, the closest direction (Q_{0j}) over the $SC_{0,j}$

426 to the point P_0 . When all $Q_{0,j}$ are known, their mean is calculated, defining the new
427 reference point P_{i+1} . If the angular distance between P_i and P_{i+1} is higher than 0.01° , it is
428 far from the solution and the process starts again using as a reference the new point P_{i+1} .
429 Otherwise, if P_i and P_{i+1} are similar (angular distance between them smaller than 0.01°),
430 this means that P_i is the closest direction to all SCs (Fig. 8) and it becomes the SCI
431 solution.

432

433 In practice, the program repeats this entire process 500 times, using each time a
434 different pseudo-sample generated by parametric bootstrapping. For this, 30 new para-
435 elements of bedding and BBC magnetization are generated at each site; the new families
436 of para-elements have the same Fisherian distribution (same k) as the input data. For
437 each of the 500 repetitions of the iterative method, a pair of para-elements (bedding and
438 BBC magnetization) is randomly chosen at each site to generate one different SC each
439 time (see section 2.2.1). Once the program has calculated 500 SCI solutions, Kent
440 (1982) statistics are applied to find the final SCI solution and the 95 % confidence
441 ellipse.

442

443 4.2. The A/n matrix approach

444

445 The program calculates the remagnetization direction using an iterative
446 approach, but in addition, it calculates the value of A/n for all possible directions (one-
447 degree grid spacing). The end result is a contour plot of A/n which allows graphical
448 analysis of the results. Both approaches must be convergent because they are based
449 upon the same assumptions and same input data. However, there are some differences
450 between them that explain why both are used in this program. The iterative approach is

451 fast and allows calculating several SCI solutions for calculating the confidence ellipse.
452 Conversely, the A/n approach takes a few minutes for calculating the A/n value for all
453 directions (32400 in total) but it provides a contour map of A/n values which gives us
454 information about the reliability of the calculated paleomagnetic direction.

455

456 4.3 Some calculations

457

458 Except for the calculation of the d value and the apical angle of the SCs, pySCu
459 uses an angle conversion for the rest of the calculations. The different elements
460 presented in previous sections can be calculated by regular spherical trigonometry but
461 due to the different situations regarding possible relationships between elements we
462 decided to do the calculations starting from a 90° rotation of the reference system and
463 consequently of all elements (the strike of the bed $-t$, SC, paleomagnetic vectors, etc.)
464 around an axis perpendicular to the trend and in a clockwise sense (looking to $t+90^\circ$).
465 Then: (i) the strike t becomes the vertical axis, and (ii) all elements placed the same SC
466 will have the same inclination. In this way, all calculations can be done by scalar
467 subtraction of declinations or inclinations (Fig. 10).

468

469 4.3.1. α value and Q coordinates

470

471 As indicated in the previous sections, α_j is the minimum angular distance
472 between P and a particular SC $_j$ and it is measured along a great circle (GC) having the
473 same strike as the SC. After the above mentioned 90° rotation of the cone axis, the plane
474 represented by this great circle becomes vertical with the same declination as P (Fig.

475 10a) and therefore the angle α corresponds to the difference in inclination between the P
476 and M vectors (in absolute value).

477

478 Q_j is defined as the intersection between the great circle that contains P and
479 whose strike is t . Therefore, after the rotation, the inclination of Q_j and M_j , on one side,
480 and the declination of P_j and M_j , on the other, will be the same (Fig. 10a).

481

482 4.3.2. *Paleodip calculation*

483

484 The paleodip is the dip of the bed when the remagnetization occurred. When the
485 remagnetization direction is finally calculated, P becomes the reference for this
486 particular bed (the remagnetization direction) and Q_j becomes the BFD (best fit
487 direction), the theoretical paleomagnetic direction of the site at the moment of the
488 remagnetization.

489 Since the actual dip of the beds is the angular distance (measured on the SC)
490 between the BBC and ATBC paleomagnetic directions, the paleodip (ϕ) is the angle
491 between BFD and ATBC paleomagnetic direction (Fig. 10b). This angle can be
492 calculated from the dihedron between the planes defined by 1) the horizontal vector
493 corresponding to the strike of the bed and the BFD for each plane on one side, and by 2)
494 the bedding strike and the ATBC vector on the other. After the 90° rotation of the
495 reference system, this calculation is simpler because it equals the angular difference of
496 the declinations between ATBC and BFD vectors.

497 Some considerations regarding the relationship between the declination of the
498 BFD and ATBC directions must be taken into account. According to the strike of the
499 bed of the example shown in Fig. 10b, point 1 (ATBC₁) agrees with a bed whose

500 paleodip is between the present day paleodip and the horizontal (i.e. the pre- and post-
501 remagnetization tilts have the same sense, see section 2.2), whereas point 2 (ATBC₂)
502 illustrates a bed whose paleodip has the opposite sense than the actual dip. This is
503 important because the paleostrike (according to the RHR, right hand rule) will be the
504 same than the strike for ATBC₁ but for ATBC₂ it will be the strike plus 180°. The
505 program considers these situations for restoring the bed in the proper way.

506

507 **5. Conclusions**

508

509 When dealing with synfolding remagnetizations, the SC methods has several
510 applications, such as performing detailed reconstructions of the attitude of each bed at
511 the time of the remagnetization, calculating the local direction of the remagnetization or
512 evaluating the presence of vertical axis rotations. All in all, one of the most important
513 applications of the SC methods is that it allows graphical analysis of paleomagnetic
514 datasets, avoiding possible “black-box” effects.

515 Application of parametric bootstrap allows us to assess the propagation of the
516 error coming from the bedding and the paleomagnetic data. Working in this way it is
517 possible to calculate the remagnetization direction together with its confidence ellipse.

518 Here the pySCu software, written in Python 2.7, for direct application of
519 different SC applications is presented. It shows the advantage of being user-friendly,
520 fast and easy, allowing a broader use of the SCI method in the paleomagnetic
521 community, specifically applied to magnetotectonic studies using synfolding
522 remagnetizations.

523

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525

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531 comments and suggestions of the reviewers Bernard Henry and Emilio L. Pueyo, which
532 have helped to improve the SC methods and constrain their application limits.

533

534 **Figure captions**

535

536 Fig. 1. (a) A small circle (SC) associated with one paleomagnetic site is defined by the
537 strike of the bedding (t) and by the direction of the magnetization (M) and therefore it
538 can be parametrized by t and the apical angle (Ap) of the SC which is equal to the angle
539 between the magnetization and strike vectors. Working in a unit sphere, Ap can be
540 defined by its cosine d . (b) α is the minimum angular distance between the given
541 direction P and the SC_M and is defined as the angle between P and Q, the latter being
542 the intersection between the SC_M and the great circle that contains P and t .

543

544 Fig. 2. Lower hemisphere, equal area projections showing the basis of the SCI method.
545 (a) Paleomagnetic dataset showing the paleomagnetic directions (before bedding
546 correction, BBC) and their respective SCs. (b) The parameter A/n is the sum of all α_j
547 normalized by the number of sites and can be calculated for the directions susceptible to
548 be the remagnetization direction. (c) A/n contour plot. The remagnetization direction
549 corresponds with the minimum value of A/n (SCI solution). The ratio mr/me (Waldhör

550 and Appel, 2006) between the real and the possible number of intersection is also
551 indicated. Paleomagnetic data come from remagnetized limestones (see supplementary
552 data)

553 Fig. 3. (a) A/n contour plots obtained from three examples of SCI solution (star) from
554 three different distributions of 20 SCs with different degree of concentricity. The
555 calculated SCIs solutions (small black points; i.e. different solutions considering the
556 uncertainty coming from bedding and paleomagnetic data) and their 95% confidence
557 ellipses and statistical parameters (Kent, 1982). (b) Equal area projections showing the
558 three corresponding SC distributions and the best fit directions (BFD). 95 % confidence
559 circle (Fisher, 1953) and 95% confidence ellipse (Kent, 1982) corresponding to the 20
560 BFDs are depicted for comparison. Statistical parameters α_{95} and maximum and
561 minimum semi-angles (η_{95} and ζ_{95}) are also indicated. The used paleomagnetic dataset
562 can be found in the supplementary material.

563 Fig. 4. Equal area projection showing the SCs and the best fit directions (BFD) of the
564 same dataset shown in Fig. 2, in which some data (dashed SC) have been artificially
565 rotated 50° according to a clockwise vertical axis rotation. Note that there are two
566 concentrations of intersections corresponding with both populations easily identifiable
567 by visual inspection. However, the contour plot of A/n shows a unique relatively well
568 defined SCI solution. This is not correct because it is calculated from two datasets with
569 different intersections as can be recognized in the SC distribution. In any case, by way
570 of example of how to show the calculated SCI solution, it is shown together with the
571 statistical parameters (η_{95} and ζ_{95} are the major and minor semi-angles according Kent -
572 1982- and A/n is the parameter introduced by Waldhör and Appel -2004-). The used
573 paleomagnetic dataset can be found in the supplementary material.

574

575

576 Fig. 5. Different examples of paleodip restorations depending of relationship of timing
577 between tilting and acquisition of the remagnetization: (a), (b) and (c) show synfolding
578 remagnetizations with different tilting histories, (d) and (e) show pre-folding and post-
579 folding remagnetization respectively. Each situation illustrates the relationship between
580 bedding and paleomagnetic direction with a 3D sketch and in equal area projection.
581 Red, blue and green correspond respectively with BBC, BFD and ATBD paleomagnetic
582 directions. In equal area projection, solid symbols are represented in the lower
583 hemisphere and hollow symbols in the upper one; note that the reference direction has
584 negative inclination.

585 Fig. 6. Schmidt projection of a set of SCs showing the symmetry of the SCs between the
586 upper and lower hemispheres and hence the two possible remagnetization direction
587 having the same declination but opposite inclinations could be right.

588 Fig. 7. Possible different workflows (w1, w2, and w3) within the pySCu_calc.py
589 module.

590 Fig. 8. Example of the output plots from pySCu_draw.py. (a), (b), (c) show the SCs and
591 BBC, BFD and ATBC paleomagnetic directions respectively. (d) Contour plot of A/n,
592 the different calculated SCI solutions and their 95% confidence zone. Paleomagnetic
593 data from Soto et al. (2011).

594 Fig. 9. Workflow followed by pySCu using the iterative approach. Given an initial
595 direction P_0 , the program starts the process with the calculation of all Q_{0j} points, and the
596 mean of the calculated Q_{1j} directions (the Q_{1j} mean being transferred to the new point

597 P_1). In each iteration the angle between P_i and P_{i+1} is calculated. The iteration process
598 goes on until the angle is lower than 0.01° . This process is repeated n times (500 by
599 default) using a different para-dataset of SCs for calculating the different SCI solutions
600 with which the 95 % confidence zone is calculated.

601 Fig. 10. (a) Equal area projection showing, as in Figure 1, the relationship between P ,
602 M , Q and α (abbreviations are the same than in previous figures and in the text). In the
603 box, the calculations performed for calculating the α value and the Q coordinates after
604 the clockwise rotation of the elements looking to $t+90$. (b) After the same clockwise
605 rotation the paleodip (ϕ) can be calculated as a difference between declinations.
606 Different possibilities exist depending on whether the sense of tilting between the pre-
607 and post-remagnetization tilting is the same or opposite (elements 1 and 2 respectively).

608

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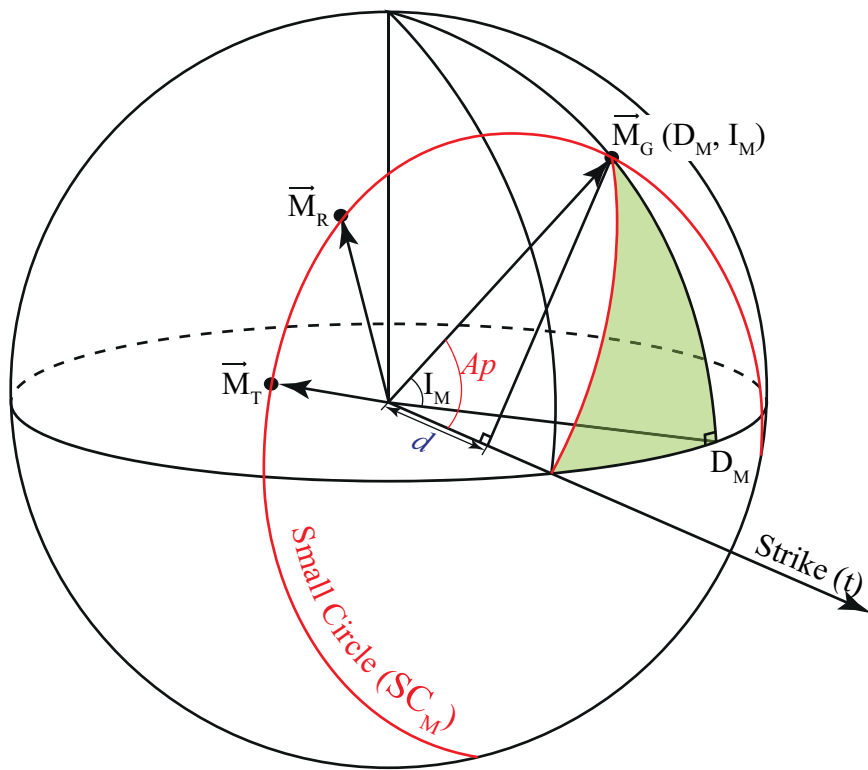
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(a) Parameters of one SC



\vec{M}_G : In situ magnetization vector

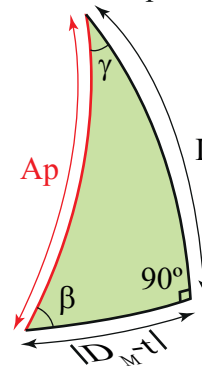
\vec{M}_T : ATBC magnetization vector

\vec{M}_R : Remagnetization vector

SC_M : Small circle associated with \vec{M}

Ap : Apical angle of the SC

d : Cosine of the Ap



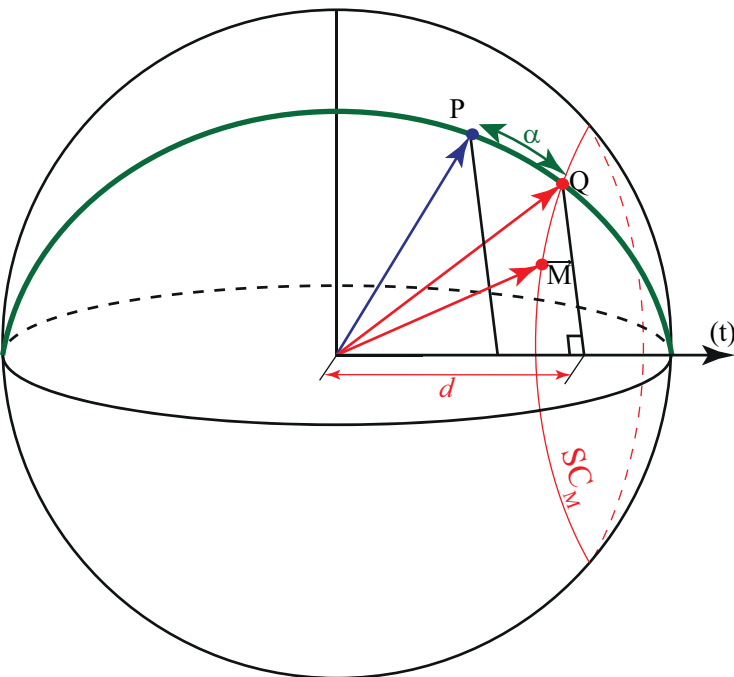
$$d = \cos Ap$$

$$d = \cos (D_M - t) \cos I_M$$

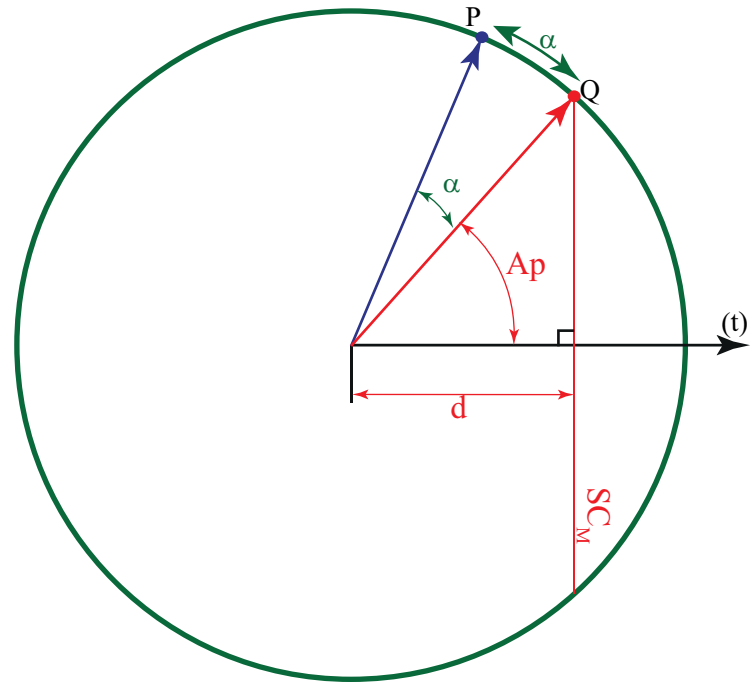
(b) P, Q and angular distance (α) between P and SC

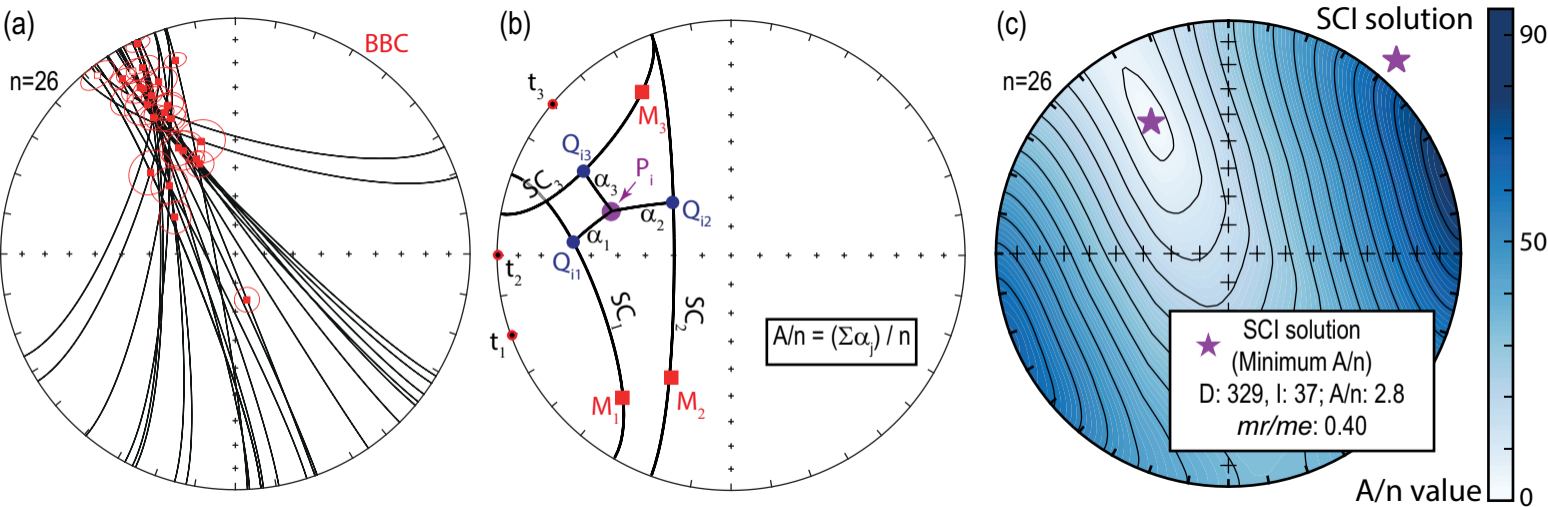
SC_M : Small circle whose axis is 't' and contains \vec{M}

Q: nearest point between P and SC_M

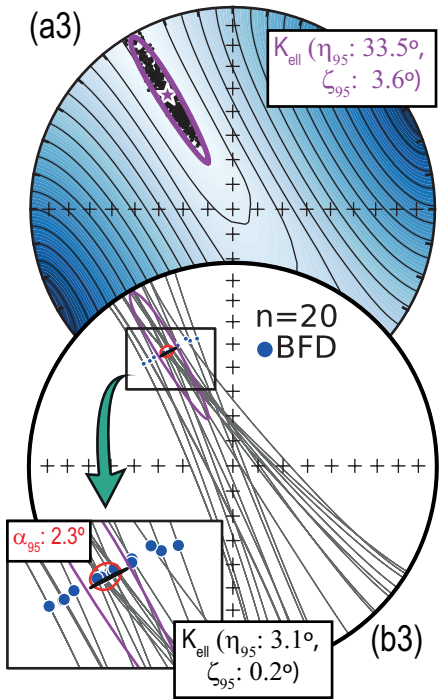
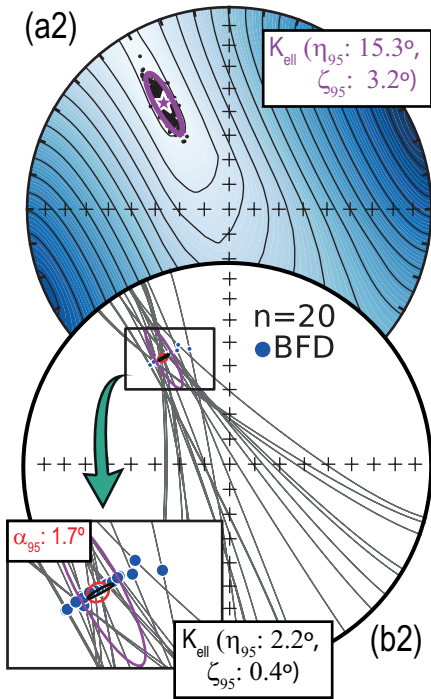
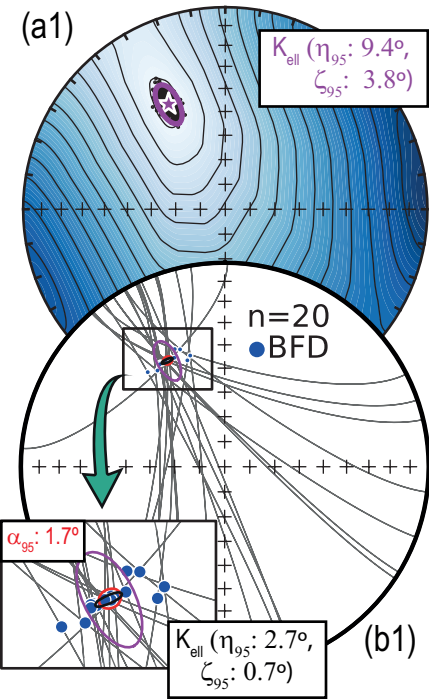


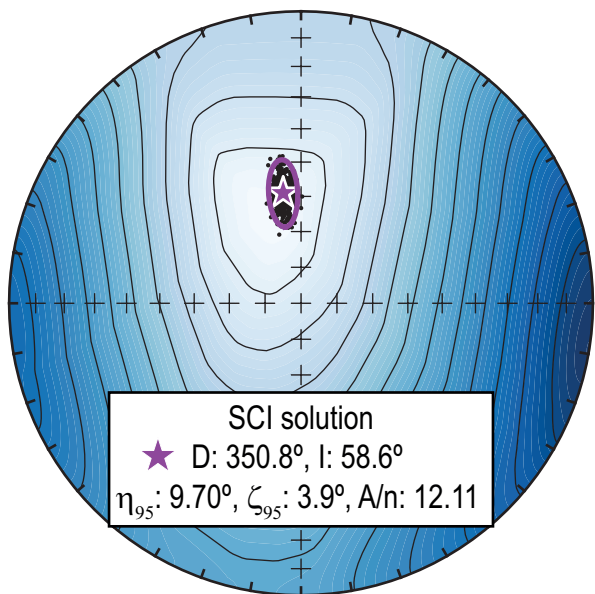
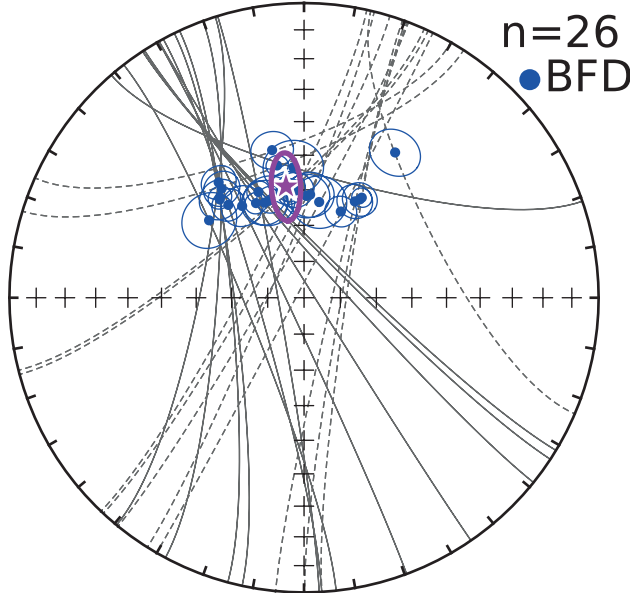
Looking perpendicular to the great circle in which P and strike are (the green one)





Increasing the concentricity of the SCs





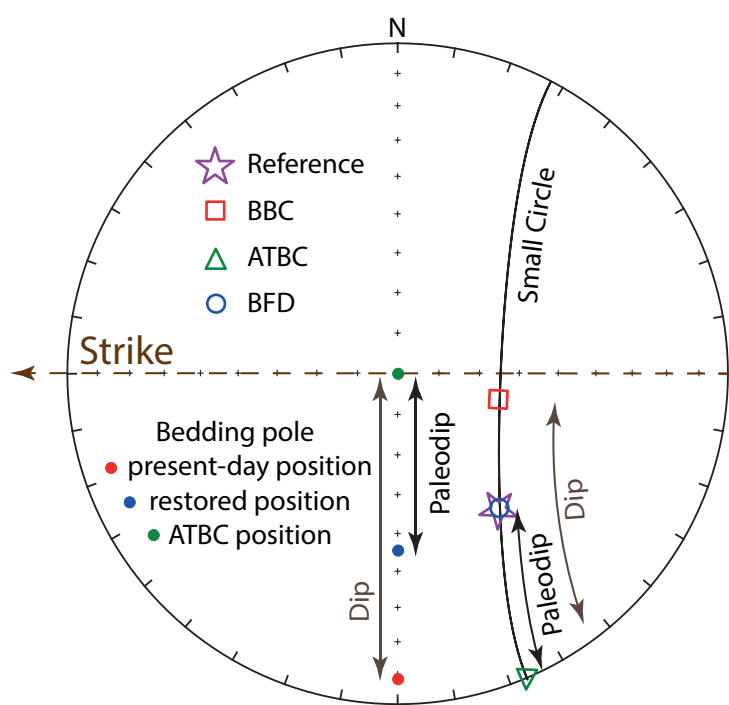
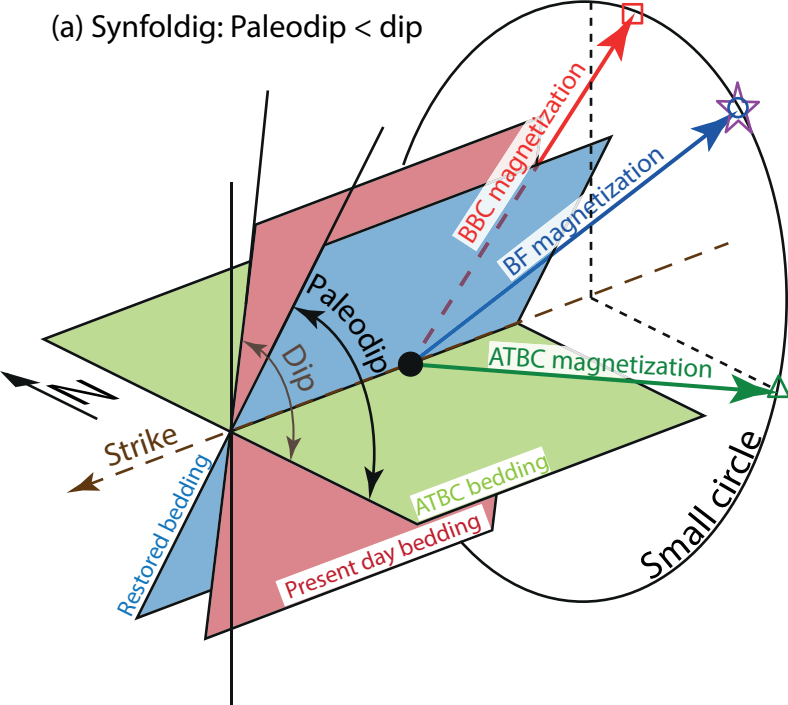
mr/mp=0.38; ● SCIs solutions (n=500)



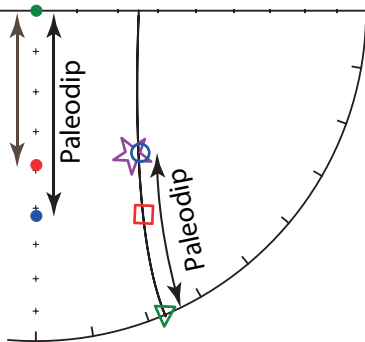
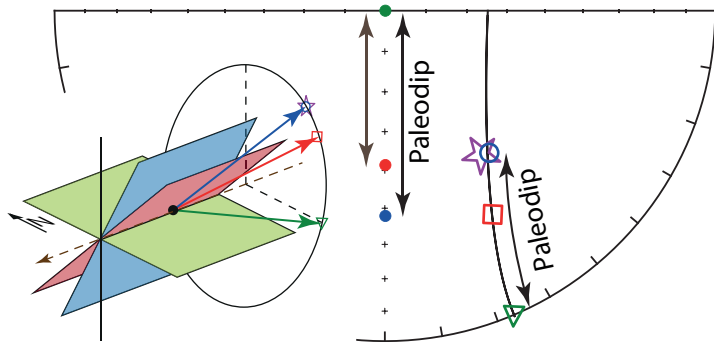
10 17 24 31 38 45 52 59 66

A/n value (11.2-69.1)

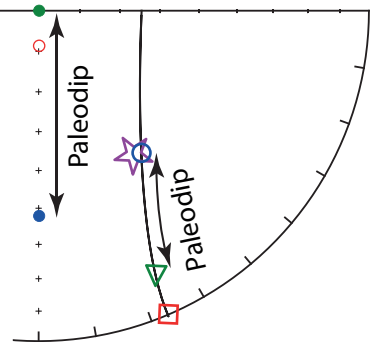
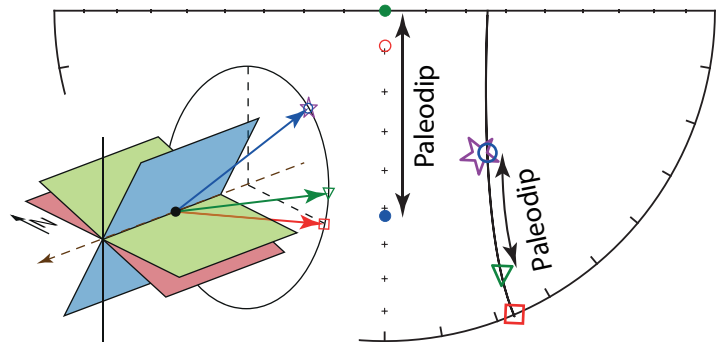
(a) Synfoldig: Paleodip < dip



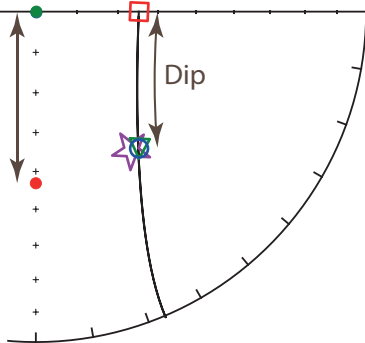
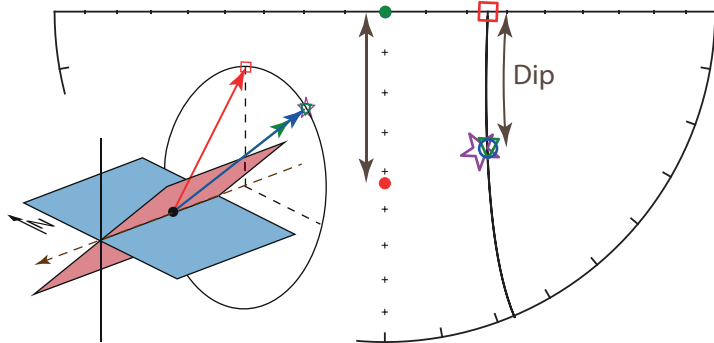
(b) Synfoldig: Paleodip > dip



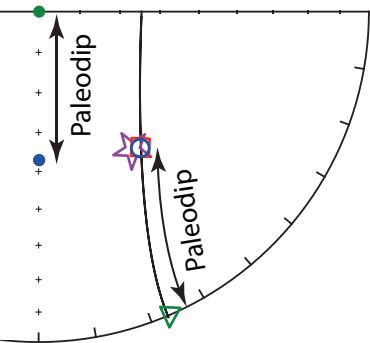
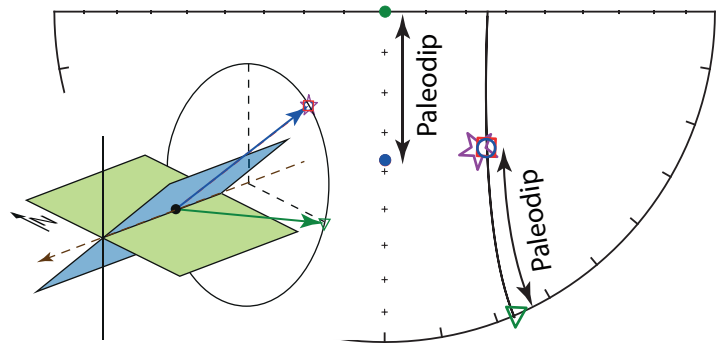
(c) Synfoldig: Change of dip sense



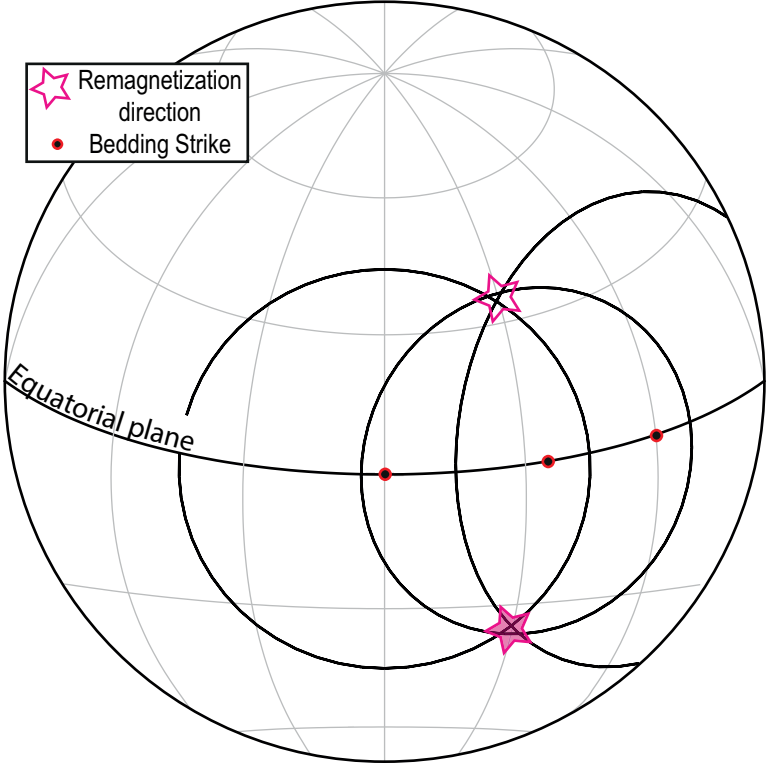
(d) Prefolding: Paleodip = 0°

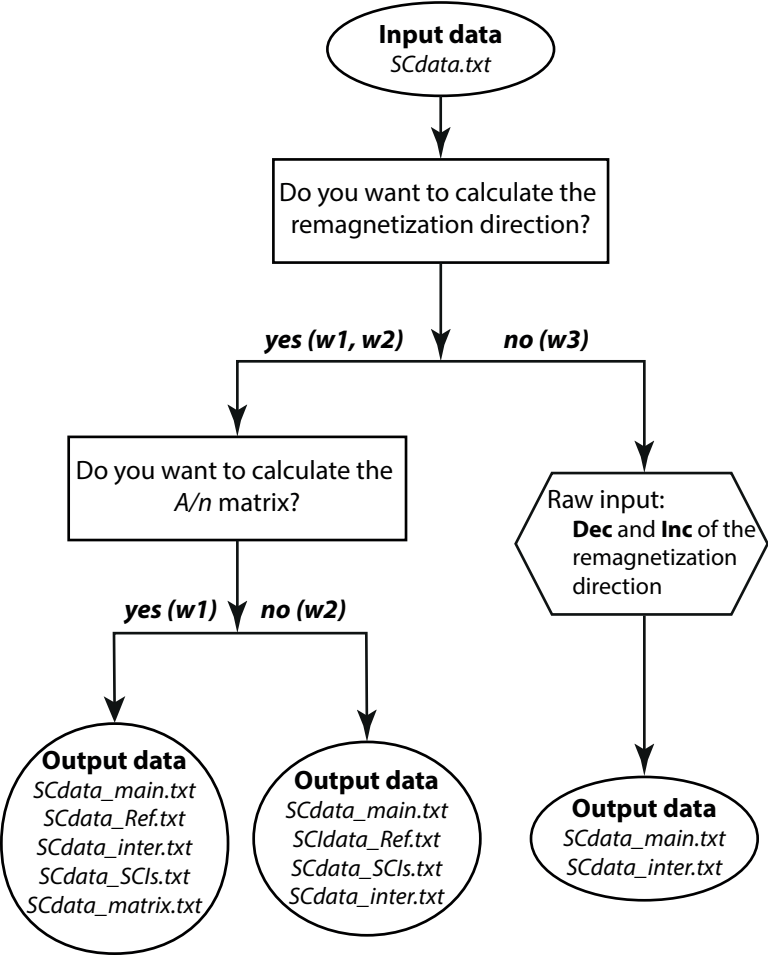


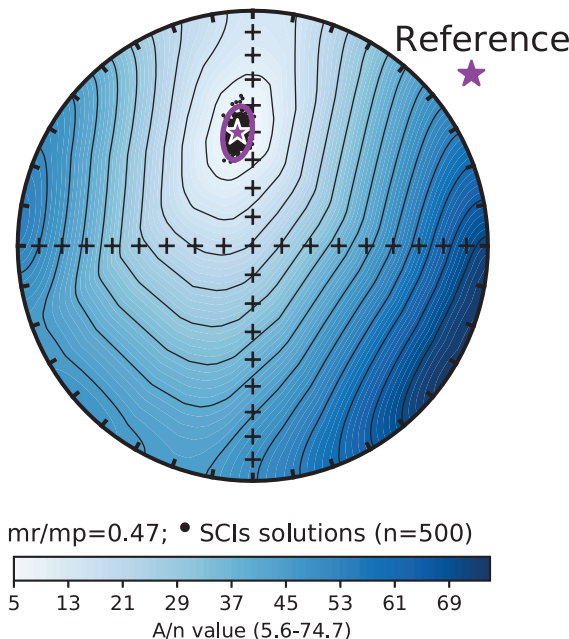
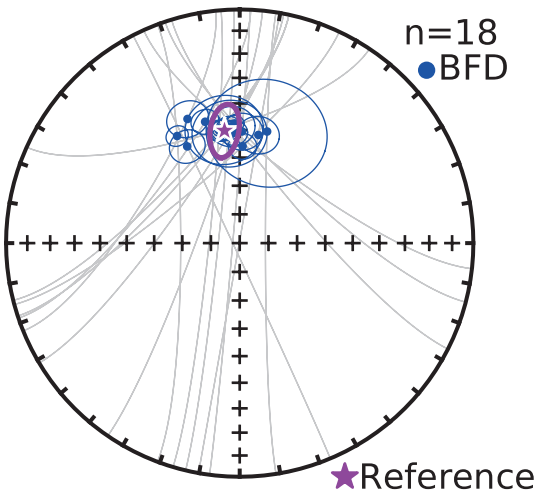
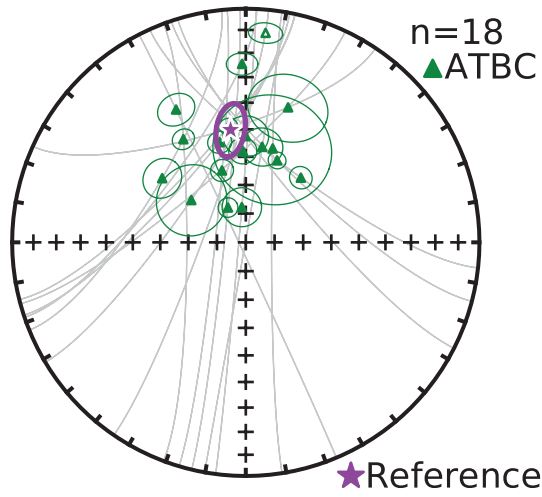
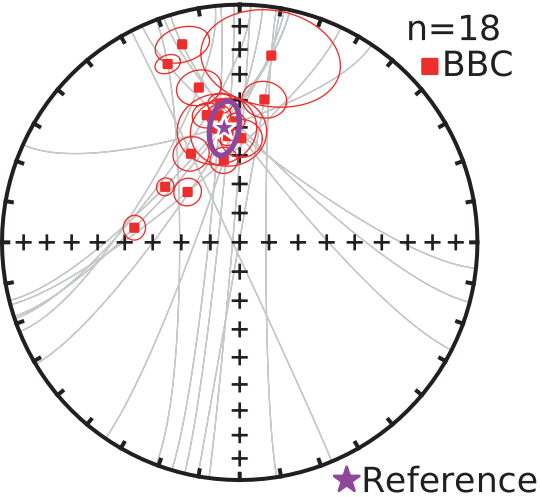
(e) Postfolding: Paleodip = dip



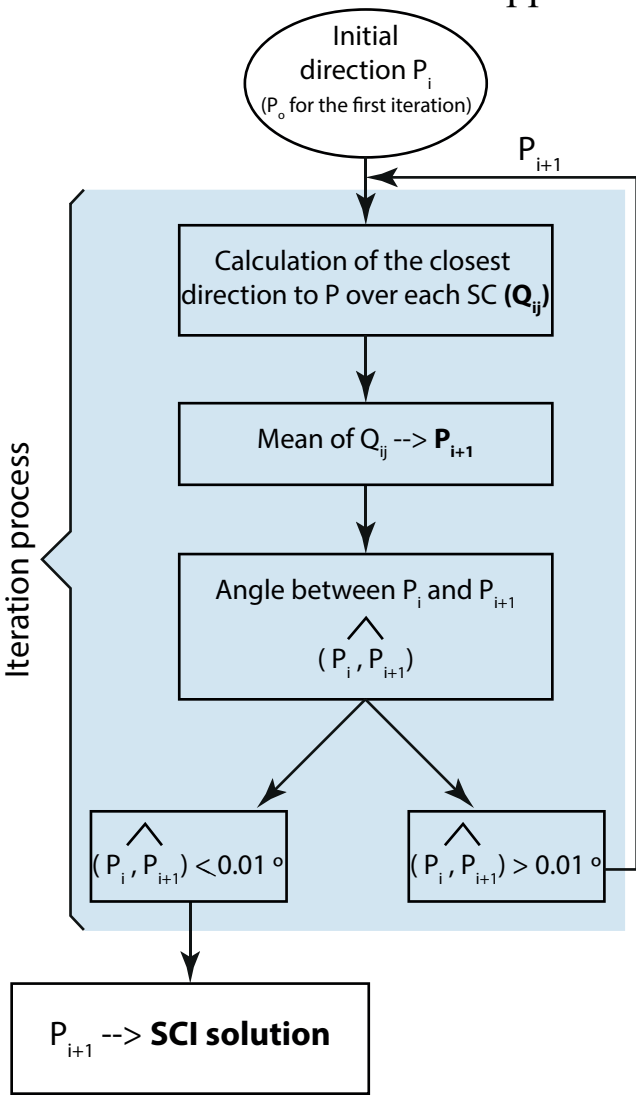
- ☆ Remagnetization direction
- Bedding Strike



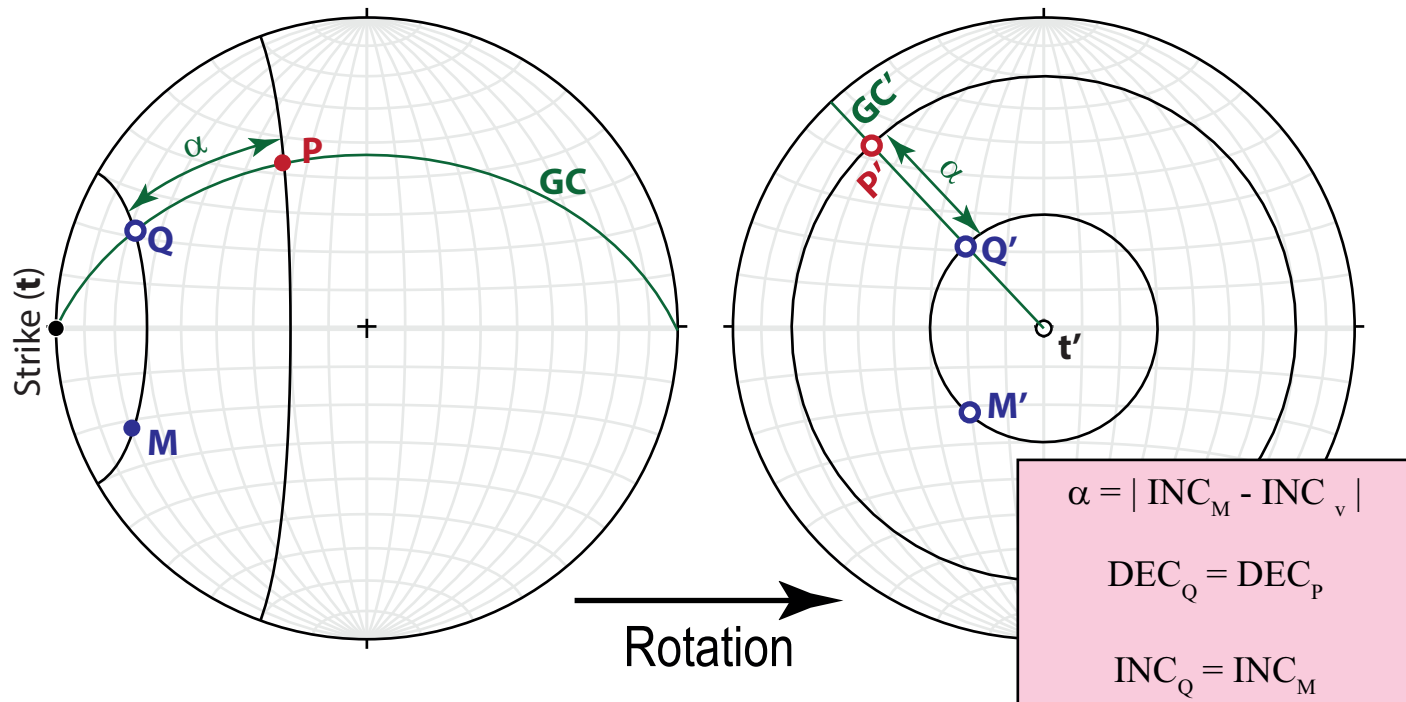




Workflow of the iterative approach



(a) α value and Q coordinates calculation



(b) Paleodip (ϕ) calculation

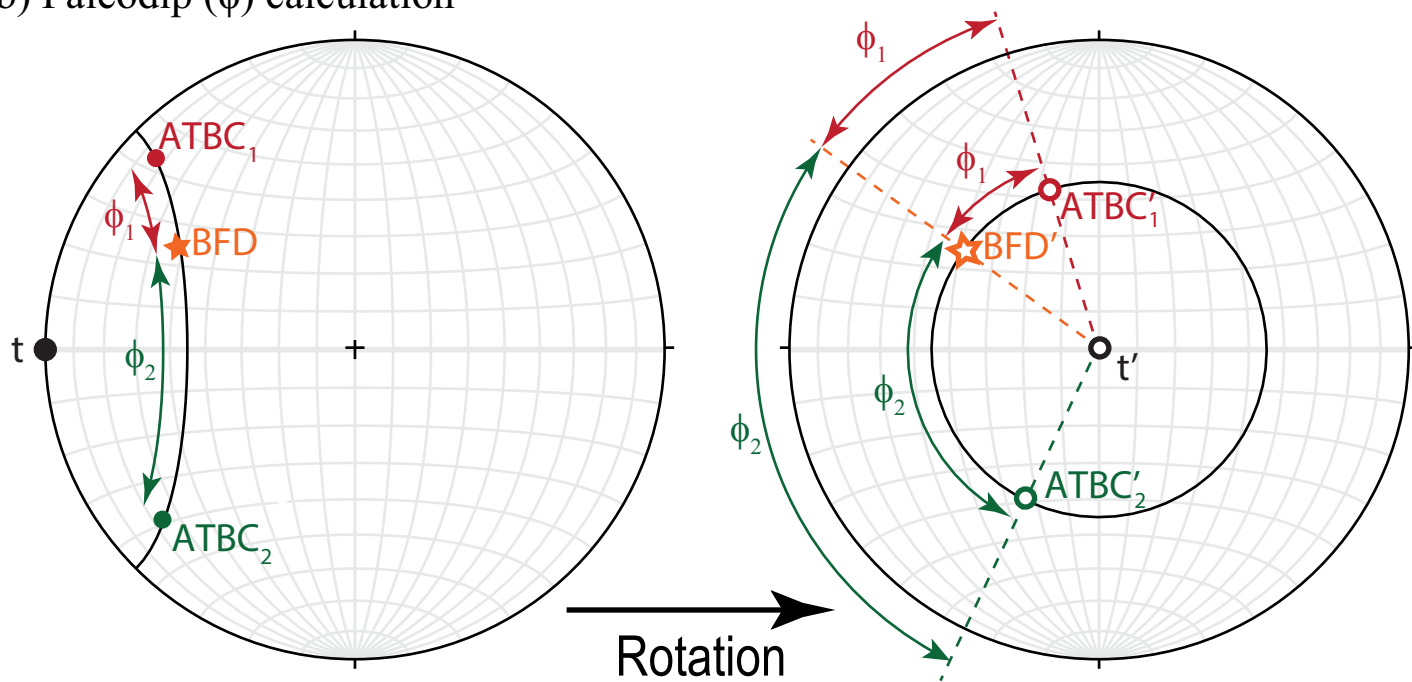


Table. 1. Example of input data file. Remember that this must to be a comma separated text file. SITE: name of the site; rem D / rem I: in situ (BBC) declination and inclination of the remanence. alpha95 and kappa: semi-angle of the cone of confidence α_{95} and k parameter (Fisher, 1953) associated to the paleomagnetic direction; Dipdir / Dip: Dip direction and dip of the bedding; k_bed: k parameter (Fisher, 1953) associated to the bedding.

SITE	rem D	rem I	alpha95	kappa	Dipdir	Dip	k_bed
St01	300.6	62.1	3.2	300.6	321	55	120
St02	348	27	3.9	202.7	270	21	120
St03	268	27	4.6	146.0	310	84	120

Data

Original data coming from Calvin et al. (2017), JSG, doi: 10.1016/j.jsg.2017.02.009

Data of Figure 2

Site	Dec_GEO	Inc_GEO	a95	k	DipDir	Dip	k_bed
AG02	329	32,9	4,5	219,4	344	0	150
AM01	335,5	31,3	4,9	130,1	4	17	150
AM02	335	2	3,2	293,6	175	60	150
AM03	342,7	15	3,1	316,6	170	53	150
AM04	334,5	36,6	4,7	138,6	191	22	150
AM06	327,1	12,4	3,8	185,9	134	32	150
AM07	331,7	47,7	6,3	114	318	26	150
AM09	333,2	49,3	7	120,3	315	13	150
AM12	313,8	48,6	7,6	54,1	338	24	150
AM13	330,7	20,8	3	350,9	148	34	150
AM14	301,1	65,4	5,6	65,4	353	46	150
AM15	343	48,6	7,9	50,4	285	22	150
AM16	330,1	19,7	5,7	139,9	155	36	150
SK01	333,4	33,4	6,7	82,8	103	61	150
SK05	315,9	56,8	6,4	76,7	333	48	150
SK06	325,9	-21,2	6,2	94,8	160	72	150
SK07	329,5	27,3	7,4	57,2	160	14	150
SK08	322,2	-4,6	5	144,3	158	49	150
SK09	332,1	25	3,3	335,8	180,1	16	150
SK10	338,4	56,3	4,7	141,5	320	30	150
SK11	165,7	73,7	4,3	167,7	338	74	150
SK12	333,4	33,4	2,9	366,1	20	0	150
SK14	333,4	12,6	4,7	140	180,1	64	150
SK15	335,9	21,1	5,5	102,7	202	41	150
SK16	337,8	54	2,7	404,8	318	18	150
SK17	330,6	-12	4,8	159	143	55	150

Data of Figure 3a

Site	Dec_GEO	Inc_GEO	a95	k	DipDir	Dip	k_bed
AM06	327,1	12,4	3,8	185,9	134	32	150
AM07	331,7	47,7	6,3	114	318	26	150
AM09	333,2	49,3	7	120,3	315	13	150
AM12	313,8	48,6	7,6	54,1	338	24	150
AM13	330,7	20,8	3	350,9	148	34	150
AM16	330,1	19,7	5,7	139,9	155	36	150
DP07	90,7	79,2	1,6	1178,8	325	70	150
DP10	321,9	31,2	5,7	115,1	333	71	150
IC03	85	87,4	7,9	59	338	66	150
IC51	337,9	25,3	4,4	136,6	139	18	150
OU07	333	13,2	8,5	82,4	160	80	150
SK03	349,8	66,2	8,1	56,4	339	75	150
SK05	315,9	56,8	6,4	76,7	333	48	150
SK06	325,9	-21,2	6,2	94,8	160	72	150
SK07	329,5	27,3	7,4	57,2	160	14	150
SK08	322,2	-4,6	5	144,3	158	49	150

Data

SK10	338,4	56,3	4,7	141,5	320	30	150
SK11	165,7	73,7	4,3	167,7	338	74	150
SK16	337,8	54	2,7	404,8	318	18	150
SK17	330,6	-12	4,8	159	143	55	150

Data of Figure 3b

Site	Dec_GEO	Inc_GEO	a95	k	DipDir	Dip	k_bed
AM03	342,7	15	3,1	316,6	170	53	150
AM06	327,1	12,4	3,8	185,9	134	32	150
AM09	333,2	49,3	7	120,3	315	13	150
AM13	330,7	20,8	3	350,9	148	34	150
AM14	301,1	65,4	5,6	97,5	353	46	150
DP02	253,3	70,2	4,3	166,7	350	60	150
DP04	320,5	52	6,8	68,1	355	14	150
DP06	328	48,4	6,6	70,4	303	59	150
DP10	321,9	31,2	5,7	115,1	333	71	150
DP11	323,4	36,1	3,7	219,5	305	51	150
IC48	328,4	2,9	5,5	119,9	161	51	150
IC50	334,6	30,4	3,1	273,1	128	10	150
SK05	315,9	56,8	6,4	76,7	333	48	150
SK06	325,9	-21,2	6,2	94,8	160	72	150
SK07	329,5	27,3	7,4	57,2	160	14	150
SK09	332,1	25	3,3	335,8	180	16	150
SK10	338,4	56,3	4,7	141,5	320	30	150
SK11	165,7	73,7	4,3	167,7	338	74	150
SK14	333,4	12,6	4,7	140	180	64	150
SK17	330,6	-12	4,8	159	143	55	150

Data of Figure 3b

Site	Dec_GEO	Inc_GEO	a95	k	DipDir	Dip	k_bed
AM01	335,5	31,3	4,9	130,1	4	17	150
AM02	335	2	3,2	293,6	175	60	150
AM06	327,1	12,4	3,8	185,9	134	32	150
AM09	333,2	49,3	7	120,3	315	13	150
AM10	329,8	38,6	8,6	114,2	288	34	150
AM15	343	48,6	7,9	50,4	285	22	150
AM16	330,1	19,7	5,7	139,9	155	36	150
DP01	194,8	62,5	6,4	75,5	355	71	150
DP03	314,7	60,3	5	144,4	1	25	150
DP04	320,5	52	6,8	68,1	355	14	150
DP09	332,1	16,4	4,1	185,7	124	78	150
DP11	323,4	36,1	3,7	219,5	305	51	150
SK13	296,5	66,7	5,7	96,2	13	62	150
OU01	319,8	42,8	7,4	57,5	228	30	150
OU06	337	26,5	8,3	45,2	188	15	150
SK01	333,4	33,4	6,7	82,8	103	61	150
SK05	315,9	56,8	6,4	76,7	333	48	150
SK07	329,5	27,3	7,4	57,2	160	14	150
SK11	165,7	73,7	4,3	167,7	338	74	150

Data

SK14 333,4 12,6 4,7 140 180 64 150

Data of Figure 4

Site	Dec_GEO	Inc_GEO	a95	k	DipDir	Dip	k_bed
AG02	329	32,9	4,5	219,4	344	0	150
AM01	335,5	31,3	4,9	130,1	4	17	150
AM02	335	2	3,2	293,6	175	60	150
AM03	342,7	15	3,1	316,6	170	53	150
AM04	334,5	36,6	4,7	138,6	191	22	150
AM06	327,1	12,4	3,8	185,9	134	32	150
AM07	331,7	47,7	6,3	114	318	26	150
AM09	333,2	49,3	7	120,3	315	13	150
AM12	313,8	48,6	7,6	54,1	338	24	150
AM13	330,7	20,8	3	350,9	148	34	150
AM14	301,1	65,4	5,6	97,5	353	46	150
AM15	343	48,6	7,9	50,4	285	22	150
AM16	330,1	19,7	5,7	139,9	155	36	150
rotated_	23,4	33,4	6,7	82,8	153	61	150
rotated_	5,9	56,8	6,4	76,7	23	48	150
rotated_	15,9	-21,2	6,2	94,8	210	72	150
rotated_	19,5	27,3	7,4	57,2	210	14	150
rotated_	12,2	-4,6	5	144,3	208	49	150
rotated_	22,1	25	3,3	335,8	230,1	16	150
rotated_	28,4	56,3	4,7	141,5	10	30	150
rotated_	215,7	73,7	4,3	167,7	28	74	150
rotated_	23,4	33,4	2,9	366,1	70	0	150
rotated_	23,4	12,6	4,7	140	230,1	64	150
rotated_	25,9	21,1	5,5	102,7	252	41	150
rotated_	27,8	54	2,7	404,8	8	18	150
rotated_	20,6	-12	4,8	159	193	55	150