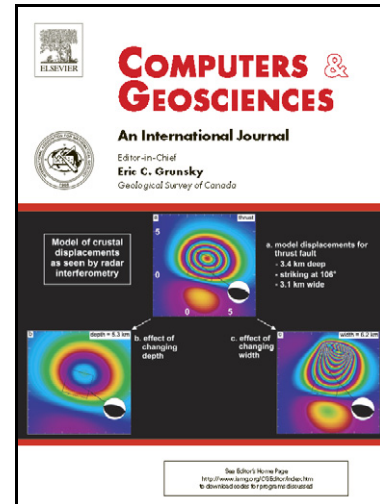


Orientation domains: A mobile grid clustering algorithm with spherical corrections

Joana Mencos, Oscar Gratacós, Mercè Farré, Joan Escalante, Pau Arbués, Josep Anton Muñoz



www.elsevier.com/locate/cageo

PII: S0098-3004(12)00223-3
DOI: <http://dx.doi.org/10.1016/j.cageo.2012.06.021>
Reference: CAGEO2953

To appear in: *Computers & Geosciences*

Received date: 4 October 2011
Revised date: 25 June 2012
Accepted date: 26 June 2012

Cite this article as: Joana Mencos, Oscar Gratacós, Mercè Farré, Joan Escalante, Pau Arbués and Josep Anton Muñoz, Orientation domains: A mobile grid clustering algorithm with spherical corrections, *Computers & Geosciences*, <http://dx.doi.org/10.1016/j.cageo.2012.06.021>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting galley proof before it is published in its final citable form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

1 **Orientation domains: A mobile grid clustering algorithm with spherical**
2 **corrections**

3 Joana Mencos^{1*}; Oscar Gratacós¹; Mercè Farré²; Joan Escalante²; Pau Arbués¹; Josep

4 Anton Muñoz¹

5 *corresponding author. GEOMODELS Research Institute, Department of Geodynamics

6 and Geophysics, Universitat de Barcelona, Martí i Franquès s/n, 08028 Barcelona,

7 Spain, phone number: +34 934 021 373, fax number: +34 934 021 340, *e-mail address*:

8 jmencos@ub.edu (Joana Mencos)

9 ¹ GEOMODELS Research Institute, Department of Geodynamics and Geophysics,

10 University of Barcelona, Martí i Franquès s/n, 08028 Barcelona, Spain

11 ² Grup de Recerca en Aplicacions i Models Matemàtics – GRAMM, Department of

12 Mathematics, Faculty of Science, Universitat Autònoma de Barcelona, 08193 Bellaterra

13 (Barcelona), Spain

14

15 **Abstract**

16

17 An algorithm has been designed and tested which was devised as a tool assisting the

18 analysis of geological structures solely from orientation data. More specifically, the

19 algorithm was intended for the analysis of geological structures that can be approached

20 as planar and piecewise features, like many folded strata. Input orientation data is

21 expressed as pairs of angles (azimuth and dip). The algorithm starts by considering the

22 data in Cartesian coordinates. This is followed by a search for an initial clustering

23 solution, which is achieved by comparing the results output from the systematic shift of

24 a regular rigid grid over the data. This initial solution is *optimal* (achieves minimum

25 square error) once the grid size and the shift increment are fixed. Finally, the algorithm

26 corrects for the variable spread that is generally expected from the data type using a
27 reshaped non-rigid grid. The algorithm is *size-oriented*, which implies the application of
28 conditions over cluster size through all the process in contrast to density-oriented
29 algorithms, also widely used when dealing with spatial data. Results are derived in few
30 seconds and, when tested over synthetic examples, they were found to be consistent and
31 reliable. This makes the algorithm a valuable alternative to the time-consuming
32 traditional approaches available to geologists.

33 **Highlights**

- 34 - Structural data (azimuth/dip) classification into Orientation Domains
- 35 - Development of a grid-based proximity-oriented algorithm with square-error criterion
- 36 - Automatic cluster partition
- 37 - Corrections designed to improve clustering results and maintain geologic criterion

38 **Keywords:**

39 Structural analysis, bedding orientation, size-oriented clustering algorithm, shifting grid,
40 square error criterion.

41

42 **1. Introduction**

43 *1.1 Structural analysis from orientation data*

44 The representation of the geometry of geological structures is central to several resource
45 and environmental applications of geology, like the characterization of hydrocarbon
46 traps, aquifers, waste disposal and CO₂ repositories. In this scenario, an accurate
47 reconstruction is fundamental to reproduce the structures under study, and this can only
48 be achieved following a 3D approach (Zanchi et al., 2009 and references within the
49 same volume).

50 Orientation data analysis is a recognized fundamental step on the reconstruction of
51 geological structures (Ramsay, 1967; Suppe, 1985; Groshong, 2006). One of the
52 objectives of the analysis of orientation data is the discrimination of clusters. Clusters

53 are data subsets that represent portions of the structure having a characteristic
 54 orientation (i.e. dip domains, Gill, 1953; Suppe, 1983; Fernández, 2004; Groshong,
 55 2006). This approach can be useful where geological structures, and specially folded
 56 strata, can be represented as planar and piecewise features (Shaw et al., 2005;
 57 Groshong, 2006) and helpful in areas where structures are complex and/or under-
 58 sampled (Wise, 1992; Torrente, M. 2000; Fernández et al. 2004; Carrera et al 2009).
 59 Typically, clusters can be derived by following a semi manual approach (Cruden and
 60 Charlesworth, 1972; Fernández, 2004; Mencos, 2011) which summarizes as follows.
 61 The analyst selects a subgroup of orientation data from the entire data set, which is
 62 regarded as a candidate for cluster. This selection is based on spatial and geological
 63 considerations. This is followed by the inspection of scatter and density stereoplots and
 64 the study of the relationships between the eigenvectors and eigenvalues that result from
 65 the Principal Component Analysis. Stereographic projections have been traditionally
 66 used in geology to represent and analyze different types of data sets (i.e. lines or planes)
 67 at the same time and without considering their geographical position.

68 Two conditions need to be satisfied for the candidate to be accepted as a cluster:

69 a) In order to compare the eigenvalues in an objective way, Woodcock (1977)
 70 introduced a criterion, which is also referred to in Fernández (2005). The
 71 condition for a set of poles to perform the same cluster is that their first ordered
 72 eigenvalue (λ_1) is high enough in comparison with the second (λ_2) and the third
 73 (λ_3) ordered ones. This relationship can be expressed as:

$$74 \quad \lambda_1 \gg \lambda_2 > \approx \lambda_3 \approx 0 \quad (1)$$

75 b) The second condition to be satisfied is that the subgroup of poles must lie within
 76 a range of orientations, such that:

$$77 \quad u_{max} - u_{min} \leq u_0 \quad \text{and} \quad v_{max} - v_{min} \leq v_0 \quad (2)$$

78 where $u_{max}-u_{min}$ denotes the range in azimuth of the data subset, $v_{max}-v_{min}$ is the
79 range in dip within the data subset, and $[u_0, v_0]$ is a range or threshold defined by
80 the analyst, which accounts for the variability that can be expected within
81 orientation domains. This variability reflects instrumental error, geological
82 roughness (e.g. lithology, bedding, texture, etc.) and sharpness (e.g. quality of
83 exposure) of the measured feature (Cruden and Charlesworth, 1976).

84 If both conditions are met, then the cluster characterizes an orientation domain and can
85 be subsequently enlarged with other measurements. If not, other subgroups have to be
86 tested. In this way, clusters characteristic of different orientation domains are retrieved
87 by a trial and error process driven by expertise. At the end of the process, a set of mean
88 azimuth and dip values (from now on referred to as centroids) representative of each
89 planar orientation domain are obtained.

90 This approach can yield different results depending upon the analyst expertise. It is also
91 time-consuming, since it requires continued supervision and generally involves working
92 with several types of software (for example CAD, database management systems,
93 structural analysis and structural modelling applications, etc.).

94 Aimed to overcome these problems, the algorithm herein provides with a fast analysis
95 tool reading from simple ASCII text files. Interaction with user is restricted to initial
96 input parameters and the process remains essentially unsupervised. Output stands also
97 simple, with initial orientation data grouped as clusters representing planar orientation
98 domains. It is important to note that the algorithm does not consider the spatial
99 distribution of the data, hence the results do not represent structural domains.

100 Subsequent analysis leading to structural domains can be achieved by loading the output
101 data on a georeferenced 3-D visualization software. This is possible as the output data

102 preserves their original XYZ location. Then, the user needs to manually select the
103 structural domains.

104 It is noteworthy that this algorithm fits within a workflow developed for the
105 reconstruction of geological structures in 3D (Fernández, 2004; Mencos, 2011). Thus,
106 this workflow supports some aspects of the structural analysis that are not tackled by the
107 algorithm, (e.g. the definition of structural domains on site).

108 *1.2 Clustering methods*

109 The term “clustering” regards to the unsupervised classification of elements into groups,
110 called clusters. The existing standard methods for clustering can be divided into two
111 main families: hierarchical and partitioning (non-hierarchical) methods. Hierarchical
112 methods produce a nested series of partitions, while non-hierarchical methods produce
113 only one partition. Several surveys on clustering analysis are available in the literature
114 (Jain et al., 1999; Bock, H.H, 2002; Xu, R., 2005).

115 Hierarchical methods are strongly dependent on the first classification step and do not
116 have a clear criterion for the final cluster partition. Moreover, when large amounts of
117 data need to be classified, a typical method in hierarchical clustering such as the
118 dendrogram visualization becomes unpractical.

119 Computationally efficient partitioning methods try to reach an optimal partition
120 depending on a given criterion function, for instance minimizing the *square-error*
121 function (i.e. the squared distances inside the clusters). The *k*-means (MacQueen, 1967),
122 the simplest and most commonly used algorithm employing a square-error criterion,
123 tends to work well with a number of isolated and compact clusters, but this condition is
124 not guaranteed in orientation measurements. Moreover, most of the non-hierarchical
125 methods require an a priori knowledge of the number of clusters to be obtained (e.g.
126 Zhou and Maerz, 2002) and this condition is seldom met in geological studies.

127 In geological engineering, several studies exist that have been developed and used
128 clustering algorithms to classify, group and/or characterize discontinuities. Zhou and
129 Maerz (2002) and Tokhmechi et al. (2011) compare the application of some classical
130 methods (Parzen classifiers, k -means, nearest neighbor, etc.). Jimenez-Rodriguez and
131 Sitar (2006) develop a spectral clustering algorithm that combines the k -means method.
132 Nevertheless, the above mentioned methods do not impose a size restriction to the
133 cluster members, hence arbitrary cluster sizes are obtained (in contrast with the
134 orientation domains here defined, see condition (2)).
135 Thus, the above described methods will not give analogous results to the classical
136 procedure described in the previous section. For this reason an ad hoc tool for
137 automated clustering has been designed. This tool lays within the framework of the
138 grid-based clustering algorithms, although with some differences compared to others
139 existing in the literature.
140 Central to grid-based methods is that individual measurements are converted to cell
141 values. However, the existing methods merge initial calculated cells with surrounding
142 ones in function of their density (i.e. number of individual measurements within each
143 cell). These density-oriented methods are widely applied to spatial data and image
144 processing, but they are not suitable for the geometric characterization of geological
145 structures, in which the number of individual measurements does not necessarily
146 constitute a criterion for cluster partition. In fact, since data distribution is not
147 homogeneous, one orientation domain can be represented by a single data measurement.
148 On the contrary, the developed algorithm has been designed specifically with geological
149 considerations during cluster partition. Moreover, it represents a new approach that
150 merges a square-error criterion function and a grid-based but size-oriented technique, as
151 it will be detailed below.

152 2. The mobile rectangular grid algorithm with spherical correction

153 2.1 Principles and notations

154 Denoted by (\mathbf{u}, \mathbf{v}) is a pair of orientation angles (azimuth and dip respectively) with
155 spherical coordinates, where azimuth \mathbf{u} (or dip direction measured from North in a
156 clockwise direction) takes values in $[0, 360^\circ]$ and dip \mathbf{v} in $[0, 90^\circ]$ measured downward
157 from horizontal. Taking unitary radius, the orientation pairs (\mathbf{u}, \mathbf{v}) correspond to the
158 following Cartesian 3D-coordinates (X_s, Y_s, Z_s) :

$$159 X_s = \sin u \sin v, \quad Y_s = \cos u \sin v, \quad Z_s = \cos v \quad (3)$$

160 These normalized direction cosinus represent unitary vectors on the sphere, and the
161 domains separation must respect the inherent spherical geometry. Several statistical
162 techniques exist to specifically treat the distributional properties of spherical data
163 (Fisher et al., 1987), although they are not suitable when working on regular grids on
164 sphere.

165 The algorithm is based on the planar representation of orientation data considering their
166 Cartesian coordinates (azimuth against dip in a 2-axis Cartesian plot or $\mathbf{u-v}$ plot). It is
167 well known that the representation of oriented data on a $\mathbf{u-v}$ plot introduces a distortion
168 that is more accentuated towards the horizontal values (maximum distortion tends to a
169 singularity in horizontal dipoles) and invalidates the results of the clustering analysis. For
170 example, in a stereographic projection, the poles of the subhorizontal planes appear
171 clustered around the centre of the sphere, leading to the interpretation of a single
172 orientation domain. On the contrary, in the $\mathbf{u-v}$ plot data close to the horizontal appear
173 scattered in the lower part resulting in an overrepresented classification (Figure 1 A).
174 Without losing sight of the distortion problem (that can be corrected a posteriori as it
175 will be explained afterwards), the advantages of using a $\mathbf{u-v}$ plot are:

- 176 a) it facilitates the definition of a regular mesh that takes into account the range in
 177 azimuth (u_0) and dip (v_0) observed within orientation domains (and explained in
 178 the previous section 1.1). This regular mesh divides the orientations space in n x
 179 m regular cells or isometric areas defining orientation domains characterized by
 180 the $[u_0, v_0]$ range (Figure 1 B);
- 181 b) it is manageable, from a computational point of view, as opposite to spherical
 182 representations;
- 183 c) a rigid shift of an initial grid can be easily implemented.

184 With these assumptions in mind, the proposed clustering process uses the cylindrical
 185 projection (identifying continuity between 0° and 360° in azimuth, Figure 1 C, D and E).
 186 In this projection it superimposes a family of regular grids in order to find out which
 187 grid in that family best separates the orientation data. This gives a first clustering
 188 classification that is corrected later on in order to avoid singularities and correct the
 189 distortion.

190 Before going further, given below are some details about the distortion. The distortion
 191 can be numerically evaluated as follows:

192 Assuming a small rectangular $[u_0, v_0]$ cell in the planar representation with centre (U, V) .

193 The area of its spherical image can be approximated by

$$194 \quad u_0 \sin(V) \cdot v_0 \quad (4)$$

195 which is smaller than $u_0 \times v_0$ unless $v=90^\circ$. Thus, in order to guaranty spherically

196 isometric domains, the rectangular cells should be locally corrected taking

$$197 \quad u_0(V) \times v_0, \quad \text{where } u_0(V) = u_0 / \sin V \quad (5)$$

198 where V is the dip mean value for all the measurements in the cell. Thus, the size of the

199 cells corresponding to subhorizontal dips is enlarged, while the cells for vertical dips

200 remain practically unchanged. The first clustering classification is then modified by

201 merging the domains that fit all together into a new (enlarged) cell, this new cell being
 202 centred in the redefined common centroid point. The corrections ensure that, at the end,
 203 the clusters cells are approximately of equal spherical area. These local modifications
 204 adapt the final solution to the configuration of the orientation measures and break the
 205 rigidity of the initial mesh too.

206

207 **2.2 The algorithm**

208 **2.2.1 Part I: Rigid shifting grid-based method**

209 The first part of the algorithm determines an initial partition of the orientation angles
 210 (\mathbf{u}, \mathbf{v}) into clusters. At the end, all the angle pairs within the same cluster will be close
 211 enough one to each other to satisfy condition (2). Solution is approached by applying a
 212 rigid shifting grid-based method to find a kind of optimal fitting. Each step is listed
 213 below in detail (Figure 2 a to e):

- 214 a) The algorithm reads from an ASCII file consisting in n pairs of orientation angles
 215 $(u_1, v_1), \dots, (u_n, v_n)$. Additional information in the ASCII file are geographical
 216 coordinates in UTM format (x, y, z) and polarity (defined by N as normal; I as
 217 reversed).
- 218 b) User is required to type the tolerance accepted within an orientation domain (grid
 219 width \mathbf{u}_0 ; grid height \mathbf{v}_0) and a grid mobility increment parameter (\mathbf{p}). This parameter
 220 \mathbf{p} will determine the shifting of the regular mesh at later steps.
- 221 c) The algorithm searches for horizontal data within the file ($v=0$). If horizontal data are
 222 found they are omitted in the cluster calculation and printed in a separate file as a
 223 single horizontal domain. This step prevents any division by 0 (see equation 5).
- 224 d) The algorithm generates a regular grid with grid spacing $(\mathbf{u}_0, \mathbf{v}_0)$ and grid vertex (the
 225 lower left point of the lower left cell) anchored in the origin of the coordinate system.

226 This grid separates the data into the grid cells. Given two orientation measurements
 227 (u_i, v_i) and (u_j, v_j) , if they are in the same cell, then they satisfy

$$228 \quad |u_i - u_j| \leq u_0 \quad \text{and} \quad |v_i - v_j| \leq v_0 \quad (6)$$

229 At this stage, all the measurements in a cell perform a cluster. For any cluster
 230 partition, the usual R^2 (R -square) statistic index is computed,

$$231 \quad R^2 = 1 - (\text{variability within clusters}) / (\text{total variability}) \quad (7)$$

232 where the variability is computed as the sum of the squared distances of the measures
 233 with respect to the corresponding centroid. This index is a quality criterion of fit to
 234 the particular partition. It is computed in terms of (\mathbf{u}, \mathbf{v}) , i.e. the cylindrical
 235 representation, but it works locally well on the sphere because of the small cells size.

236 e) The algorithm looks for an optimum cluster classification (based on R^2 criterion).

237 This is performed by moving rigidly the grid vertex (anchoring point) of that initial
 238 grid, both horizontally and vertically and by tiny increments of p size (user defined
 239 increment parameter). There will exist as many grid configurations as points fit
 240 within the lower left grid cell of the initial grid, depending on p parameter. Each of
 241 these new generated grids satisfies condition (2). The optimum, in this case
 242 depending on p , is reached when the rigid rectangular grid best fits the set of nodes,
 243 i.e. maximises R^2 . Notice that highest R^2 is equivalent to a minimum *square-error*
 244 *criterion function* (Jain et al., 1999). The idea of shifting a grid structure has been
 245 used by several authors for shape recognition (Ma and Chow, 2004; Chang et al.,
 246 2009).

247

248 2.2.2 The algorithm. Part II: spherical and unrigidity corrections

249 The second part of the method consists in applying a correction to the initial cluster
250 distribution (Figure 2 e), aiming to reduce the distortion and improve the obtained
251 results. The correction consists in two operations that are done simultaneously (Figure 2
252 f to h):

253 f) Spherical adaptation: This step is necessary to adapt the grid partition to the spherical
254 geometry of data (Figure 3). It consists in converting the initial (u_0, v_0) cells
255 (isometric on the Cartesian plane) to pseudo-isometric clusters on the sphere (Figure
256 3 A). As it has been pointed out previously, to correct areal distortion, the resulting
257 cell size can be rewritten as (5).

258 The new rectangular cells which size is defined by (5) are wider as they approach the
259 zero dip area. The spherically adapted clusters are not isometric any more in the
260 plane but they approximately are on the sphere. In this way, orientation domains
261 (highly) horizontal will admit a strong variation in the u component (Figure 1 A).
262 Ideally, subhorizontal nodes will be part of a single orientation domain despite of
263 their azimuth attitude.

264 g) Unrigidity correction: A pair of nodes can be close enough one to each other to be
265 part of the same orientation domain (i.e. accomplish condition (2)), but the partition
266 obtained after step (e) separates them into different clusters. This situation is related
267 to the rigidity of the mesh that cannot be adapted to the entire set of nodes. This
268 mesh rigidity can be improved through the application of a proximity criterion, so as
269 to regroup some domains originally separated during the initial calculation (Figure
270 3). This operation is performed by searching for all the initial clusters that, even
271 separated, fit entirely within a spherically adapted cell. The search is done in an
272 organized way starting by the closest centroid pair.

273 h) Final results: Output file is an ASCII data file including the location (x,y,z) of the
274 original data point; its orientation (azimuth, dip); identification number of the
275 orientation domain to which it belongs to; number of nodes within that orientation
276 domain; calculated cluster azimuth (centroid azimuth); calculated cluster dip
277 (centroid dip); distance in azimuth between the data point and the calculated cluster
278 centroid; distance in dip between the data point and the calculated cluster centroid;
279 range in azimuth within calculated orientation domain; range in dip within calculated
280 orientation domain; identification number relating the data points to the position of
281 these data points in the original file; and finally the polarity, using 0 as a normal or 1
282 as an inverse (Table 1).

283 As a summary, the designed algorithm subdivides a set of orientation data into constant
284 orientation domains, using user-defined tolerance thresholds that account for variability
285 within orientation domains. The designed approach does not require a prior knowledge
286 of the number of clusters to identify as well as their geographic location. The program
287 has been implemented in C.

288 **3. Sample synthetic experiments**

289 A set of experiments has been designed to test the capability of the algorithm. These
290 experiments consist in different synthetic geological structures, each one representing a
291 fold with a specific structural configuration. The first experiment is used to illustrate the
292 algorithm behaviour in detail (Figure 4 B and C, see Figure 5, and 6 for results). The
293 other experiments (Figure 7 and 8) represent more complex structures and are used to
294 test the algorithm response in front of different ideal situations. The objective is to
295 illustrate the relationship between the output of the algorithm and the synthetic
296 structures, i.e. the capability of the algorithm to identify representative orientation
297 domains at convenience.

298 The experiments set up has been done as follows: each structure was generated in a 3D
299 reconstruction program by creating a folded surface (with a scale of hundreds of
300 meters). After that, some roughness was added to the surface in order to mimic the
301 variability that accounts for instrumental error, natural roughness and sharpness (except
302 experiment 3, Figure 7 B). This was done using a random function ($\text{urand}(0.5, -0.5)$ in
303 meters) applied to the Z value of each node of the initial surface (Fig 4 A). As a result,
304 the final orientation of the surface triangles could vary up to $\pm 10^\circ$. Finally, a set of
305 discrete orientation values was randomly picked on the surface, aiming to represent a
306 realistic field data acquisition (Figure 4 B). Thus, the final result is a set of scattered
307 points, each of them having a particular location and orientation (x, y, z, azimuth, dip).
308 After that, the experiment set up was ready for conventional structural analysis (Figure
309 4 C).

310 In the first experiment, the generated structure corresponds to a kink-type fold including
311 six planar regions separated by sharp hinges (Figure 4 B). Fold geometry is cylindrical
312 with horizontal axis. Each of the planar regions has a characteristic orientation
313 (dip/azimuth value). The results of the conventional structural analysis are shown in
314 Figure 4 C, and are consistent with the six-region structure.

315 In the second experiment, the created structure is also a kink-type fold constituted by
316 five planar regions, within which azimuth and dip remain more or less constant (Figure
317 7 A.1). In this case fold geometry is conical with horizontal axis.

318 In the third experiment, the created structure is a smooth folded surface that represents a
319 conical fold with continuous curvature (Figure 7 B.1), i.e. it can be defined as
320 constituted by an infinite number of planar regions. In this case, dip and azimuth show a
321 progressive change that is more pronounced close to the cone apex.

322 The fourth experiment represents also a kink-type fold with cylindrical fold geometry
323 and horizontal axis. In this case, the fold has three cylindrical domains with two
324 structural trends (Figure 7 C.1).

325 Two additional experiments have been designed using the above described bi-axial
326 kink-type cylindrical fold: The fifth experiment, consisting in the selection of a data
327 subset considering only one cylindrical domain of the fourth experiment (Figure 8 A).
328 Finally, the sixth experiment, consisting in a random selection of data extracted from
329 the experiment 4 (Figure 8 B).

330 **3.1. Test results**

331 Experiment 1: The algorithm has been run nine times (T1 to T9) with different values of
332 dip range (v_θ). Azimuth threshold has been maintained constant through all tests
333 ($u_\theta=10^\circ$), as changes in strike are negligible in the designed synthetic structure. v_θ
334 ranges from 5 to 45 degrees, with an incremental value of 5 degrees in each run. Results
335 are summarized in figures 5 and 6.

336 Experiment 2: The algorithm has been run two times varying dip range ($v_\theta = 5^\circ, 15^\circ$)
337 and maintaining azimuth constant ($u_\theta=10^\circ$) to enhance the dip influence in cluster
338 identification. The second run ($u_\theta, v_\theta = 10^\circ, 15^\circ$) solved the five planar regions of the
339 synthetic structure (Figure 7 A.2 and A.3).

340 Experiment 3: The algorithm has been run two times maintaining dip range constant
341 ($v_\theta=15^\circ$) and varying azimuth range ($u_\theta= 10^\circ, 45^\circ$). The algorithm tends to separate the
342 data into narrower orientation domains as $[u_\theta, v_\theta]$ decreases. Subvertical limbs do not
343 show significant differences between runs due to very low azimuth variability in these
344 areas; in contrast, subhorizontal domains are larger as azimuth increases, due to a
345 greater variability in azimuth (Figure 7 B.2 and B.3).

346

347 Experiment 4: The algorithm has been run two times ($u_0, v_0 = 15^\circ, 15^\circ$ and $30^\circ, 15^\circ$). In
348 this case, the algorithm identified orientation domains despite their geographical
349 position (e.g. orientation domains within cylindrical domain number 2, Figure 7 C.2).
350 Greater azimuth ranges ($u_0=30^\circ$) give a fewer number of clusters in the hinge area,
351 where azimuth variability is higher (compared to the fold limbs).
352 Experiment 5: The algorithm has been run once, using the same tolerance thresholds of
353 the fourth experiment ($u_0, v_0 = 30^\circ, 15^\circ$) to compare the results. Fewer clusters were
354 found near the hinge area compared to experiment 4, due to a lower variability in
355 azimuth and dip (e.g. compare the circled areas in Figure 8 A, each one containing a
356 single cluster, in contrast with the same areas of Figure 7 C.3). This lower variability in
357 azimuth and dip can be related to a fewer amount of data.
358 Experiment 6: The algorithm has been run once with the same tolerance thresholds than
359 experiment 4 ($u_0, v_0 = 30^\circ, 15^\circ$). The use of fewer data implies less azimuth and dip
360 variability, and therefore fewer orientation domains are obtained (Figure 8 B). However,
361 the structure is well defined.

362

363 4. Discussion

364 The synthetic experiments allowed exploring the capability of the program to solve the
365 given structures with different resolutions, by varying one or both of the user-defined
366 initial parameters (dip or azimuth values). Some of the results are discussed below.
367 In the first experiment, considering that the synthetic cylindrical structure has been built
368 using six planar domains, the best solution is when the six expected domains are
369 distinguished ($u_0, v_0 = 10^\circ, 5^\circ$ and $u_0, v_0 = 10^\circ, 10^\circ$). Dip ranges greater than these values
370 produce an under-sampled structure. If the structure under study is a kink-type fold

371 conical structure (experiment 2), the application of the algorithm can also identify the
372 expected five planar regions.

373 In a real case, where the geometry of the structure under study is generally unknown,
374 there is not a unique best-fit solution, as all possible solutions would be computationally
375 correct. The best-fit orientation-domain discrimination will depend on the available
376 data, the desired resolution and the geological properties of the materials under study
377 (e.g. lithology, bedding or texture, among others) (Figure 9). Moreover, if the structure
378 could be defined as continuous, as for example in experiment 3, then the desired
379 resolution is definitely a key-factor for cluster partition. In such a case, there would be
380 as many clusters as initial data exist, because the structure is defined as smooth and
381 continuous (Figure 7 B). Ideally, there are not a finite number of planar domains that
382 define the geometry of the structure, so that the final solution depends on the analyst.

383 Initially, no geographic position is required to identify planar regions considering their
384 orientation, hence orientation data with similar values can be grouped into the same
385 cluster even if they are geographically separated (experiment 4, Figure 7.C). This can
386 give relevant information about the fold geometry and/or evolution when it is framed
387 within a reconstruction process. As the reconstruction process goes forward, it could be
388 necessary to spatially select data subsets in order to refine the results (Figure 8 A)

389 The extraction of a data set from experiment 4 by area or randomly (experiments 5 and
390 6, respectively, Figure 8) leads to similar results with small differences since initial data
391 are different. However, these differences do not prevent to obtain a correct geometry of
392 the analyzed structure.

393 A lower threshold of azimuth and/or dip range can be established, below which the
394 orientation-domain configuration will not describe the geological geometry of the
395 structure under study (Figure 10). The orientation-domain configuration below this

396 threshold would be biased by the instrumental error, geological roughness and
397 sharpness (Figure 9).

398 As the azimuth and/or dip range increases, the geometry depicted by orientation
399 domains has lower resolution, and the number of identified planar regions decreases
400 (Figure 5 and 6). At the end, there is an upper tolerance threshold such that all the
401 available data will belong to a single orientation domain (Figure 9).

402 Compared to the semi-manual approach, the designed algorithm is fast for the
403 orientation domain definition, as well as it gives objective results. This last fact is due to
404 an automatic grouping of the original data considering only the user-established initial
405 thresholds.

406 A potential alternative to our approach could be based on *quaternions* (lying in the
407 hypersphere S^3), which provide a computationally efficient way to store and rotate 3-
408 dimensional vectors (e.g. Karney, C., 2007). In Karney, C., 2007, the quaternions
409 algebra is used to solve several problems in the orientations space. In particular, they
410 describe the projection of a cubical regular grid (defined on a *tesseract* or 4-dimensional
411 cube), over the hypersphere. This results in a distorted grid with maximum distortion in
412 the corners. The implementation of this method to our context would imply projections
413 of a regular grid onto a classical sphere (S^2) causing a distortion too. The regular shift of
414 the grid would cause unchecked distortions that would not add significant improvement
415 to our implementation.

416

417 5. Conclusions

418 An algorithm is presented to automatically obtain constant orientation domains. It is
419 based on a shifting rectangular grid clustering algorithm. Three main requirements led
420 to the use of a grid-based algorithm: unknowing the number of clusters to be obtained,
421 omitting the geographic location of data during process and obtaining clusters
422 composed of close orientations.

423 The algorithm first generates data clusters from a set of orientation data. These initial
424 clusters are subsequently improved by making a deformation of the grid to adapt it to
425 the spherical geometry inherent to the orientation measurements.

426 The resulting domain classification is based on *preserve a size* criterion for the output
427 cluster orientation domains. It starts working in the angular space and then corrects the
428 distortion to be almost isomorphic on the spherical representation given by the director
429 cosinus.

430 It depends on the user parameter specifications. The accurate definition of the threshold
431 parameters is a fundamental task for the analyst. The effects of measurements accuracy,
432 the work scale, the lithology, the structural style of deformation, etc., must be taken into
433 account when defining the parameter thresholds. By testing different thresholds, the
434 computed partitions can be improved and this is controlled by the quality criteria of fit.
435 Nevertheless, before a definitive final orientation domain assignment, the output
436 domains should be plotted on a 3D representation of the terrain, where other variables
437 can be taken into account (i.e. geographic proximity, stratigraphic position or lithology,
438 among others).

439 The performed experiments conclude that the algorithm gives acceptable results on the
440 selected tolerances with respect to the data distribution, for the selected geometries.

441 The introduction of the “mobile grid algorithm with spherical adaptation and unrigidity
442 correction” speeds up the process of structural analysis and improves the existent
443 workflow for the reconstruction of geological structures (Fernández, 2004). The
444 obtaining of any output result is fast compared to the manual approach, so that the
445 algorithm can be applied multiple times with different input parameters. With such a
446 procedure, multiple possible solutions can be explored in a short amount of time, until
447 an adequate result is obtained.

448 **Acknowledgements**

449 This work has been carried out with the financial support of the Inversión Positiva de
450 Estructuras de Tectónica Salina (CGL2010-21968-C02-01) and Modelización
451 Estructural 4D (CGL2007-66431-C02-01BTE) projects. We wish to acknowledge Grup
452 de Geodinàmica i Anàlisi de Conques (2009SRG-1198), GEOMODELS Research
453 Institute and Grup de Recerca en Aplicacions i Models Matemàtics. We also wish to
454 acknowledge Paradigm for providing gOcad software, which has been used for data
455 management and visualization. The original manuscript has been improved thanks to
456 the valuable comments of two anonymous reviewers and editor Jef Caers.

457

458 **6 References**

- 459 Bock, H.H., 2002. Clustering methods: from classical models to new approaches.
460 *Statistics in transition* 5(5), 725-758.
- 461 Carrera, N. and Muñoz, J. A. and Roca, E., 2009. 3D reconstruction of geological
462 surfaces by the equivalent dip-domain method: An example from field data of the Cerro
463 Bayo Anticline (Cordillera Oriental, NW Argentine Andes), *Journal of Structural*
464 *Geology* 31(12), 1573-1585.
- 465 Chang, C-I., Lin, N.P., Jan, N-Y., 2009. An Axis-Shifted Grid-Clustering Algorithm.
466 *Tamkang Journal of Science and Engineering* 12(2), 183-192.
- 467 Cruden, D.M., Charlesworth, H.A.K., 1972. Observations on the numerical
468 determination of axes of cylindrical and conical folds. *GSA Bulletin* 83, 2019-2024.
- 469 Cruden, D.M., Charlesworth, H.A.K., 1976. Errors in strike and dip measurements,
470 *GSA Bulletin* 87, 977-980.
- 471 Fernández, O., 2004. Reconstruction of geological surfaces in 3D. An example from the
472 southern Pyrenees. PhD Dissertation, University of Barcelona, Barcelona, Spain, 321
473 pp.
- 474 Fernández, O., 2005. Obtaining a best fitting plane through 3D georeferenced
475 data. *Journal of structural geology* 27, 855-858.
- 476 Fisher, N.I., Lewis, T., Embleton, B.J.J., 1987. *Statistical Analysis of Spherical Data*.
477 Cambridge University Press, UK, 344pp.
- 478 Gill, W.D., 1953. Construction of geological sections of folds with steep limb
479 attenuation, *AAPG Bulletin* 37(10), 2389-2406.
- 480 Groshong, R.H.Jr., 2006. *3D Structural Geology: A Practical Guide to Quantitative*
481 *Surface and Subsurface Map Interpretation*. Springer-Verlag, DE, 400 pp.

- 482 Jain, A.K., Murty, M. N., Flynn, P.J., 1999. Data clustering: A review. ACM
483 Computing Surveys 31(3), 264–323.
- 484 Jimenez-Rodriguez, R., Sitar, N., 2006. A spectral method for clustering of rock
485 discontinuity sets. International Journal of Rock Mechanics and Mining Sciences 43
486 (7), 1052-1061.
- 487 Karney, C., 2007. Quaternions in molecular modeling. Journal of Molecular Graphics
488 and Modelling 25 (5), 595-604.
- 489 Ma, E.W.M., Chow, T.W.S., 2004. A new shifting grid clustering algorithm.
490 Pattern recognition 27, 503-514.
- 491 MacQueen, J. B., 1967. Some Methods for classification and Analysis of Multivariate
492 Observations. In: Proceedings of 5-th Berkeley Symposium on Mathematical Statistics
493 and Probability, Berkeley, US, California Press 1, 281-297.
- 494 Mencos, J., 2011. Metodologies de modelització i reconstrucció 3D d'estructures
495 geològiques: anticlinal de Sant Corneli – Bóixols (Pirineus Centrals). PhD Dissertation,
496 University of Barcelona, Barcelona, Spain, 277 pp.
- 497 Ramsay, J.G., 1967. Folding and Fracturing of Rocks. McGraw Hill, US, 568 pp.
- 498 Shaw, J.H., Connors, C., Suppe, J., 2005. Seismic Interpretation of Contractional Fault-
499 Related Folds: An AAPG Seismic Atlas. American Association of Petroleum
500 Geologists, Studies in Geology 53.
- 501 Suppe, J., 1983. Geometry and kinematics of fault-bend folding, American Journal of
502 Science 283, 684-721.
- 503 Suppe, J., 1985. Principles of Structural Geology. Prentice-Hall, US, 537 pp.
- 504 Tokhmechi, B., Memarian, H., Moshiri, B., Rasouli, V., Noubari, H. A., 2011.
505 Investigating the validity of conventional joint set clustering methods. Engineering
506 Geology 118 (3-49), 75-81.

- 507 Torrente, M.M., Civile, D., Martino, C., Milia, A., 2000. Assetto strutturale ed
508 evoluzione tettonica dell'area di Monte Vesole-Monte Chianello (Cilento, Appennino
509 meridionale), Bollettino della Società Geologica Italiana 119, 733-747.
- 510 Wise, D.U., 1992. Dip Domain method applied to the Mesozoic Connecticut valley rift
511 basins, Tectonics 11(6), 1357-1368.
- 512 Woodcock, N.H., 1977. Specification of fabric shapes using an eigenvalue
513 method. Geological Society of America Bulletin 88, 1231-1236.
- 514 Xu, R., 2005. Survey of clustering algorithms. IEEE Transactions on neural
515 networks 16(3), 645-678.
- 516 Zanchi, A., de Donatis, M., Gibbs, A., Mallet, J.L., 2009. Imaging geology in 3D,
517 Computers & Geosciences 35 (1), 1-3.
- 518 Zhou, W., Maerz, N.H., 2002. Implementation of multivariate clustering methods for
519 characterizing discontinuities data from scanlines and oriented boreholes. Computers
520 and Geosciences 28 (7), 827-839.
- 521

522 **Figure Captions**

523 Figure 1. Stereographic (equal-area lower hemisphere stereoplots) versus Cartesian
 524 representation of orientation data. A. Differences between stereographic and $u-v$ plot
 525 representations of a subhorizontal data set. B. Regular mesh superimposed to the $u-v$
 526 plot and defined by $n \times m$ cells in function of the defined u_0 and v_0 values. White nodes
 527 are azimuth-dip angle pairs. Black node is the mean azimuth and dip value (centroid).
 528 C. Stereographic projection of a set of nodes. D. $u-v$ planar plot representation of the
 529 same data set. E. $u-v$ cylindrical representation with 0° and 360° identification.

530 Figure 2. Flow-chart describing the procedure followed by the algorithm. See text for a
 531 more detailed explanation of **a** to **h** steps.

532

533 Figure 3. Corrections (gray lines) applied to the initial cluster distribution (black lines).
 534 Black dots denote the initial clusters centroids without corrections. Grey dots denote the
 535 new clusters centroids after corrections. Sphericity correction: note that the influence of
 536 this correction is important in lower dips (A) and small in higher ones (B), because
 537 when $v \approx 90^\circ$, then $\sin(v) \approx 1$. Rigidity correction: Performed to join a pair of nodes
 538 close enough to be part of the same orientation domain. This correction affects in the
 539 same way all considered nodes, independently of their position in the Cartesian plot (A
 540 and B).

541 Figure 4. Initial setup for the first sample synthetic experiment. A. Illustration of how
 542 roughness is applied to the original folded surface using a random function. This
 543 function modifies Z values of the surface nodes and consequently the orientation of the
 544 surface triangles. B. Six-region kink-type fold geometry and the set of points randomly
 545 picked on the surface (represented as oriented disks). C. Stereographic representation
 546 (equal-area lower hemisphere stereoplot) and associated statistics of the data set

547 showing a cylindrical distribution and a six-region structure. E1, E2 and E3 denote the
 548 resulting eigenvectors (E1 representing the highest one and E3 the lowest).

549 Figure 5. Test results on the synthetic data set for the first experiment: $u-v$ plot (left) and
 550 perspective view (right). To the left, blue corresponds to data points and red
 551 corresponds to centroids. To the right, the coloured disks correspond to the orientation
 552 points picked on the surface, coloured in function of the cluster assignment (note that
 553 colour is assigned randomly in each run). C1 to C6 indicate the orientation domains.

554 Test results separated from A to D in function of the given tolerance thresholds: T1: ν_0
 555 = 5° ; T2: $\nu_0 = 10^\circ$; T3: $\nu_0 = 15^\circ$; T4: $\nu_0 = 20^\circ$; T5: $\nu_0 = 25^\circ$; T6: $\nu_0 = 30^\circ$; T7: $\nu_0 = 35^\circ$; T8:
 556 $\nu_0 = 40^\circ$; T9: $\nu_0 = 45^\circ$.

557 Figure 6. Summary of the obtained results. Setup parameters are: T1: $\nu_0 = 5^\circ$; T2: ν_0
 558 = 10° ; T3: $\nu_0 = 15^\circ$; T4: $\nu_0 = 20^\circ$; T5: $\nu_0 = 25^\circ$; T6: $\nu_0 = 30^\circ$; T7: $\nu_0 = 35^\circ$; T8: $\nu_0 = 40^\circ$; T9:
 559 $\nu_0 = 45^\circ$. Obtained orientation domains are: T1-T2; 6 clusters; T3-T6: 4 clusters; T7: 3
 560 clusters; T8-T9: 2 clusters.

561 Figure 7. Set up configuration and test results for experiments 2, 3 and 4, corresponding
 562 respectively to a conical kink-type fold (A), conical smooth fold (B) and bi-axial
 563 cylindrical kink-fold (C). For each experiment, 1 shows the stereographic projection of
 564 initial data, 2 shows the test results in a 3D perspective view (disks are coloured in
 565 function of cluster assignment), 3 shows the test results plotted on a $u-v$ plot (with
 566 initial data points and clusters centroids).

567 Figure 8. Test results for experiments 5 and 6. A. Experiment 5: Cylindrical kink-type
 568 fold extracted from one sector of the experiment 4. B. Experiment 6: Data subset
 569 randomly selected from experiment 4 configuration (Bi-axial kink-type fold geometry is
 570 preserved). See text for more detailed explanations.

571 Figure 9. Plot of the number of obtained clusters in function of ν_θ . The number of
572 identified planar regions decreases for larger ν_θ thresholds. Note that the orientation
573 ranges below a certain threshold can be attributed to an inherent error in the orientation
574 domain separation.

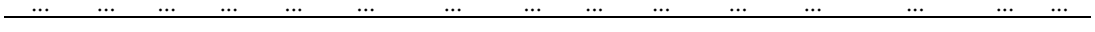
575 Figure 10. Orientation domains identified for experiment 1 when using a tolerance
576 threshold below the resolution of the designed experiment. A. Cluster distribution in a
577 perspective view ($\nu_\theta = 1$). Disks are coloured in function of cluster assignment. B.
578 Number of planar domains obtained using small dip thresholds.

579 **Table Captions**

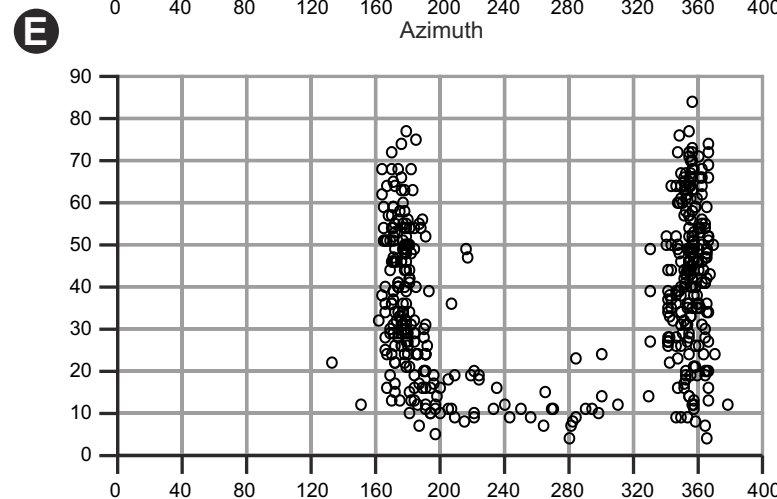
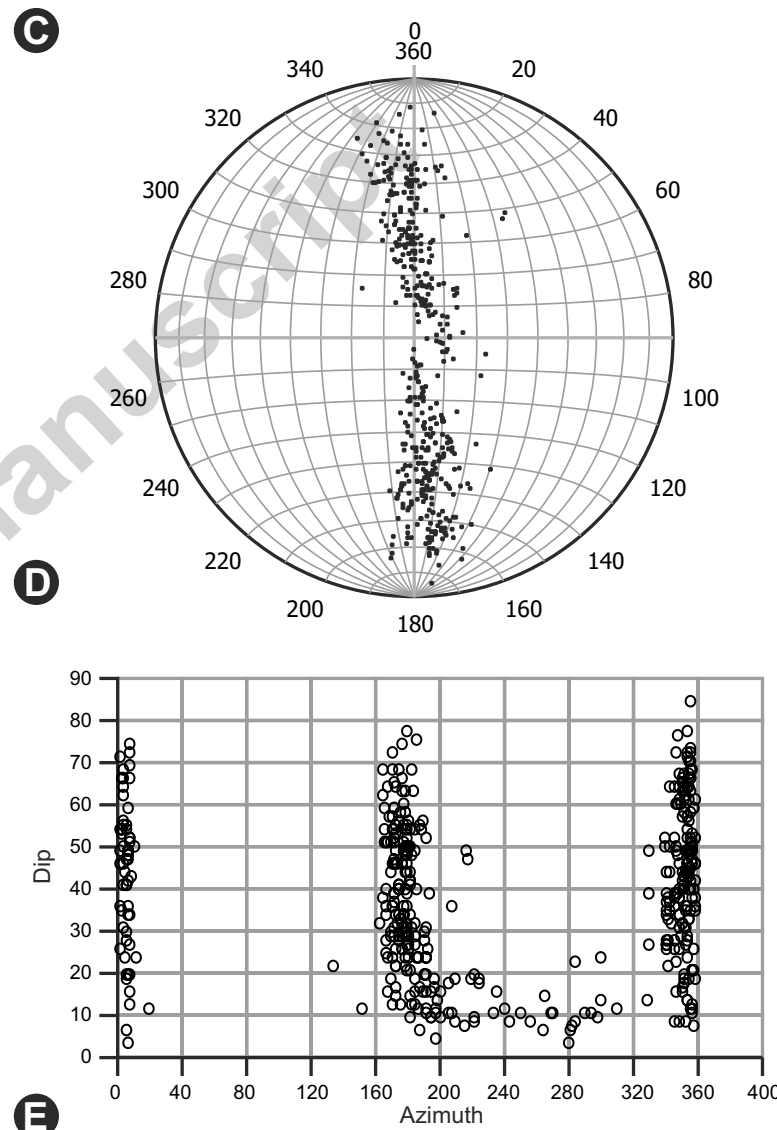
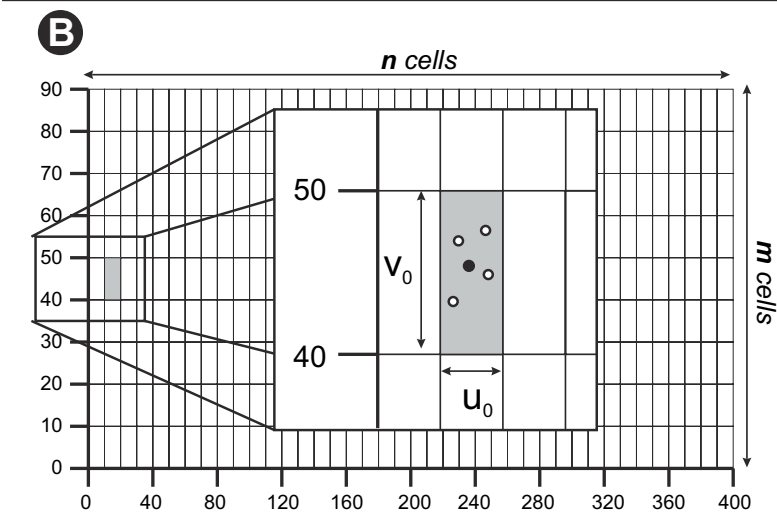
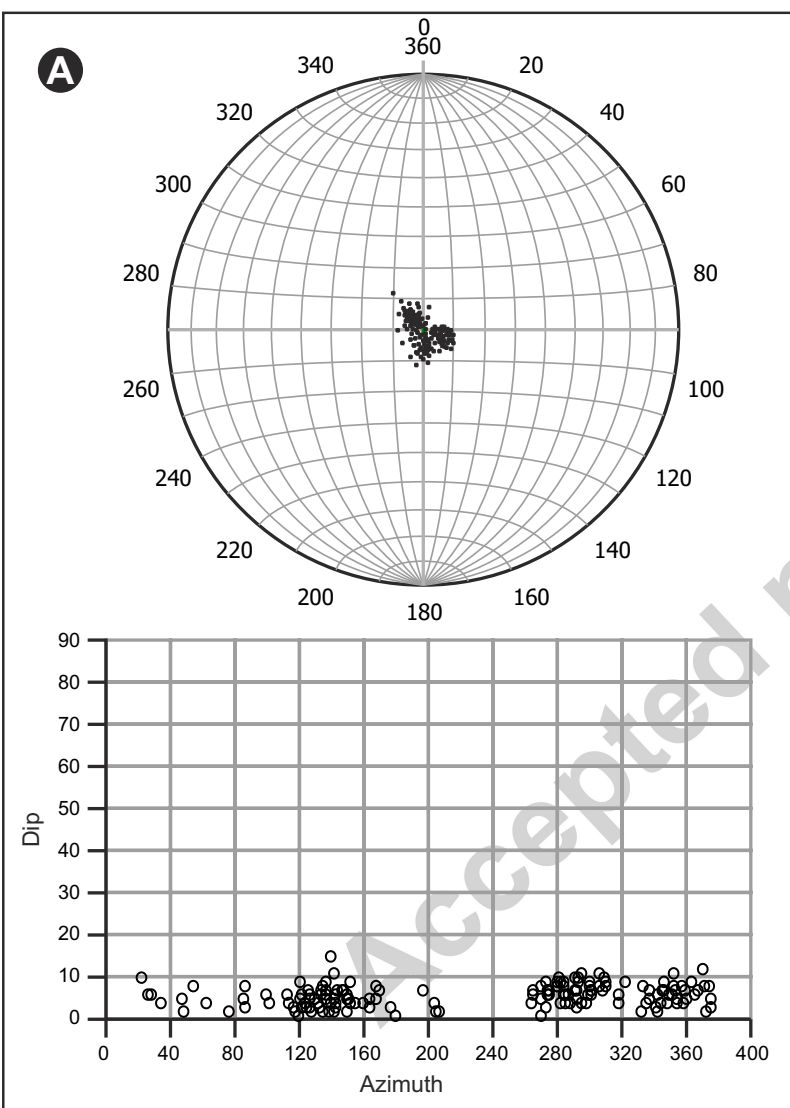
580 Table 1. Example of output results. The table represents part of an output ASCII file
581 showing 26 initial data grouped into two orientation domains (the first one with 11 data
582 and the second one with 15) and the given related parameters for each point: x, y and z
583 coordinate, azimuth and dip values, orientation domain assignation, number of points
584 included in the domain, azimuth and dip of the calculated centroid, distance in
585 orientation between the point and the corresponding centroid, orientation domain range,
586 identification number for the point and polarity.

587

x coord	y coord	z coord	Original Azimuth	Original Dip	Ori- entation domain nr.	Nr. of data in the domain	Clus- ter Azi- mut- h	Clus- ter Dip	Diffe- rence with Az	Diffe- rence with Dip	Az rang- e in dom- ain	Dip range in domain	Id nr.	Pol- arit- y
1305	978.	0.9	120.				119.	34.						
2.57	91	9	0	34.0	1	11	91	51	0.084	0.510	3.10	3.15	1	0
1310	107	1.7	120.				119.	34.						
8.65	0.17	6	3	33.6	1	11	91	51	0.431	0.878	3.10	3.15	3	0
1301	902.	4.4	119.				119.	34.						
1.77	78	3	4	32.9	1	11	91	51	0.500	1.600	3.10	3.15	4	0
1314	113	5.2	121.				119.	34.						
4.60	1.14	0	0	33.0	1	11	91	51	1.088	1.510	3.10	3.15	5	0
1304	971.	1.0	120.				119.	34.						
4.95	58	7	9	33.4	1	11	91	51	1.023	1.102	3.10	3.15	6	0
1299	887.	3.7	120.				119.	34.						
8.95	07	0	0	35.0	1	11	91	51	0.086	0.489	3.10	3.15	0	0
1306	100	1.6	119.				119.	34.						
7.70	8.26	7	6	36.0	1	11	91	51	0.279	1.537	3.10	3.15	2	0
1309	103	10.	119.				119.	34.						
0.45	5.17	63	6	35.5	1	11	91	51	0.267	0.943	3.10	3.15	7	0
1300	885.	10.	117.				119.	34.						
3.62	65	98	9	36.1	1	11	91	51	2.009	1.551	3.10	3.15	8	0
1306	991.	5.3	120.				119.	34.						
0.47	69	7	2	34.5	1	11	91	51	0.288	0.021	3.10	3.15	9	0
1312	109	6.3	120.				119.	34.						
4.01	9.41	2	0	35.6	1	11	91	51	0.055	1.059	3.10	3.15	10	0
1301	960.	23.	119.				120.	55.						
2.43	04	05	0	54.3	2	15	50	03	1.501	0.764	4	3	22	0
1299	910.	24.	123.				120.	55.						
1.01	55	46	0	53.0	2	15	50	03	2.499	2.028	4	3	14	0
1302	949.	8.3	120.				120.	55.						
6.41	38	6	1	54.8	2	15	50	03	0.407	0.203	4	3	11	0
1312	114	18.	120.				120.	55.						
9.09	0.78	37	1	56.0	2	15	50	03	0.430	0.972	4	3	13	0
1309	109	23.	120.				120.	55.						
4.94	4.37	57	0	54.6	2	15	50	03	0.490	0.393	4	3	15	0
1308	106	16.	119.				120.	55.						
1.93	5.88	65	0	55.8	2	15	50	03	1.501	0.732	4	3	16	0
1310	109	11.	120.				120.	55.						
2.51	9.76	21	2	54.9	2	15	50	03	0.349	0.137	4	3	17	0
1305	100	12.	120.				120.	55.						
0.96	6.83	98	0	56.0	2	15	50	03	0.481	0.972	4	3	20	0
1306	102	4.8	119.				120.	55.						
3.53	1.47	1	9	54.8	2	15	50	03	0.562	0.272	4	3	23	0
1300	922.	4.5	120.				120.	55.						
9.72	46	5	2	55.9	2	15	50	03	0.272	0.828	4	3	25	0
1311	110	13.	121.				120.	55.						
1.80	9.74	44	0	54.8	2	15	50	03	0.499	0.245	4	3	12	0
1305	102	20.	121.				120.	55.						
5.29	5.48	66	0	55.0	2	15	50	03	0.499	0.022	4	3	18	0
1308	104	0.7	121.				120.	55.						
0.15	7.18	3	0	54.6	2	15	50	03	0.499	0.384	4	3	19	0
1311	110	3.7	122.				120.	55.						
7.86	8.04	8	0	55.7	2	15	50	03	1.499	0.644	4	3	21	0
1301	937.	8.9	121.				120.	55.						
4.93	44	1	0	55.3	2	15	50	03	0.499	0.298	4	3	24	0



Accepted manuscript



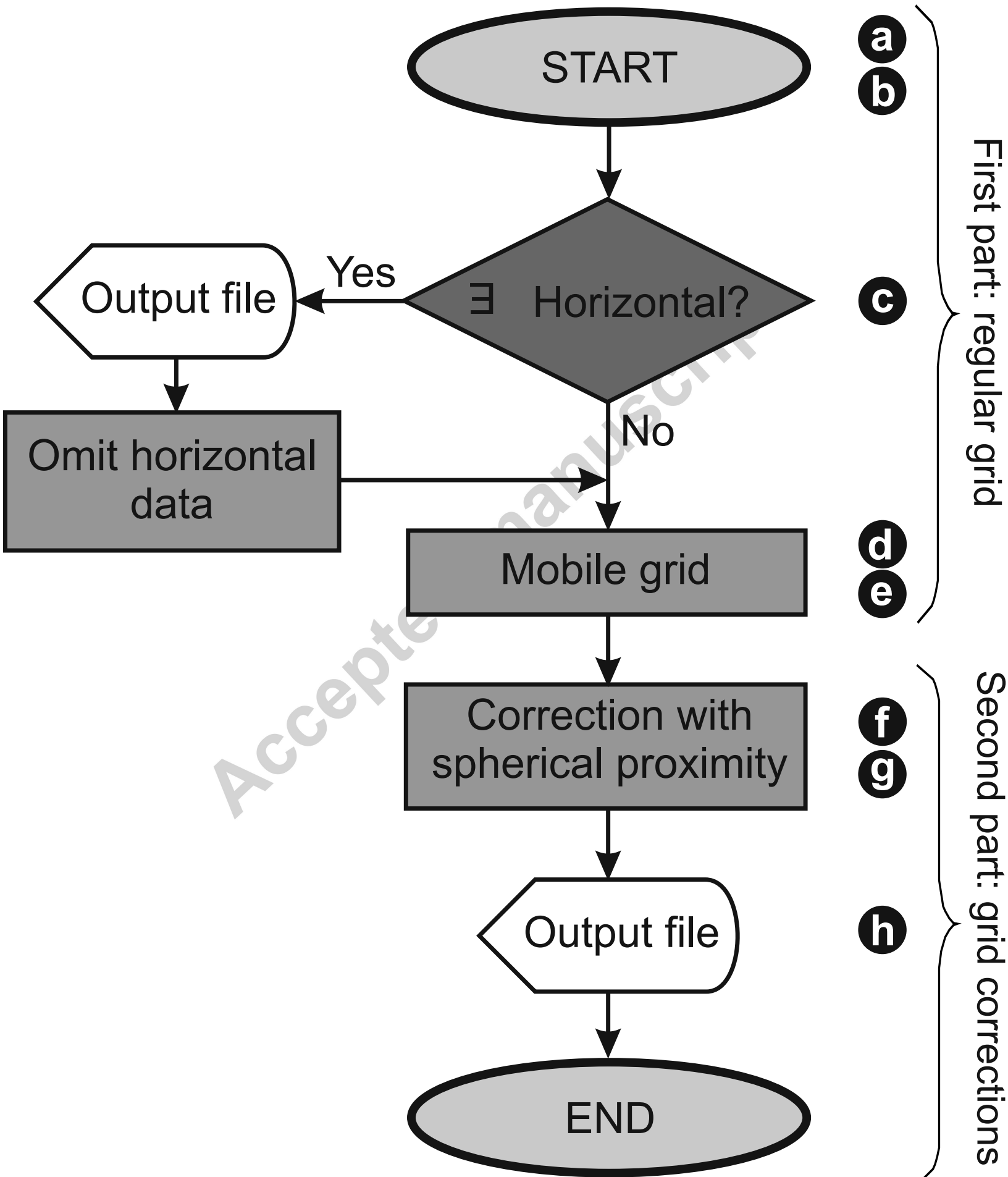
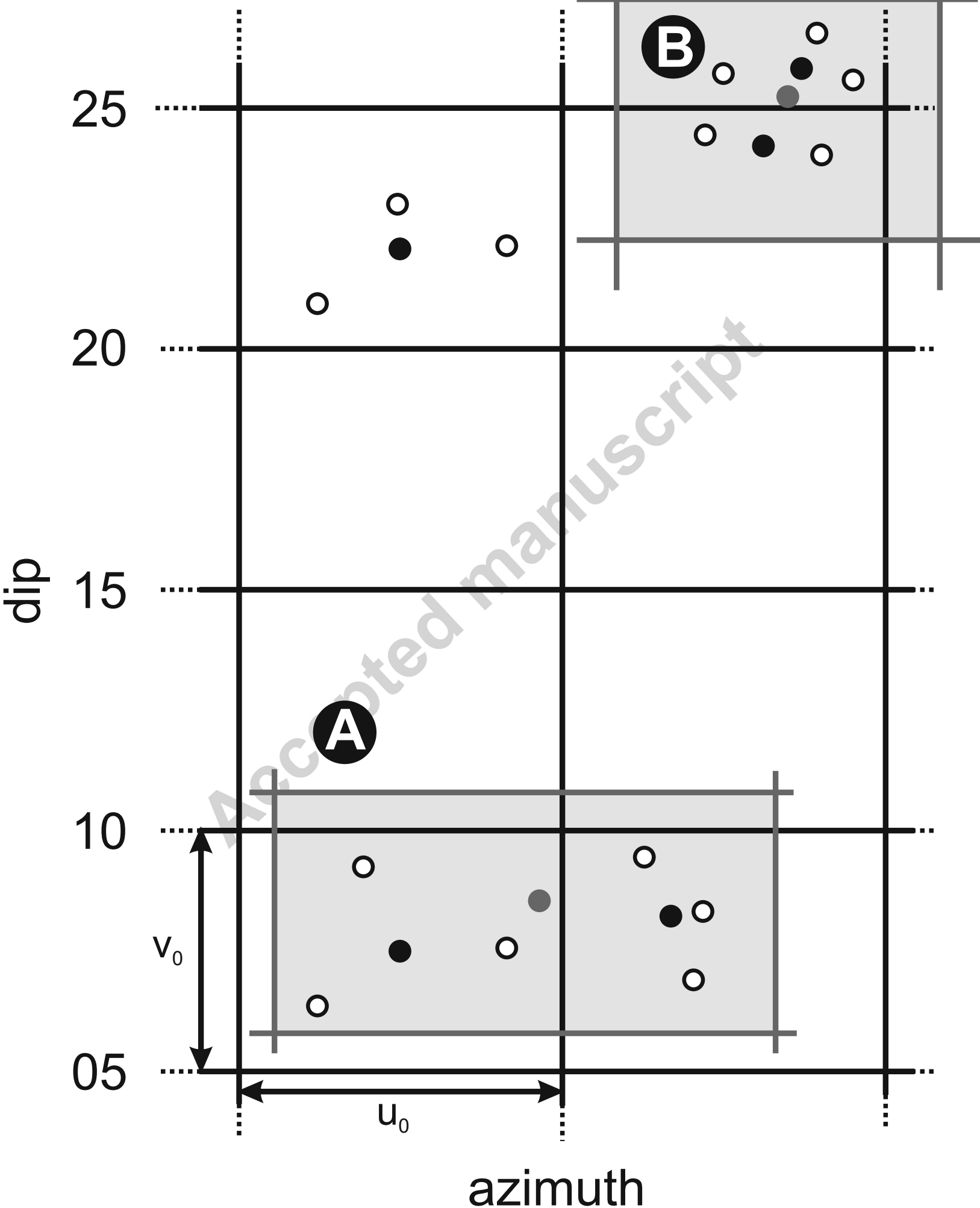


Figure 3



Accepted manuscript

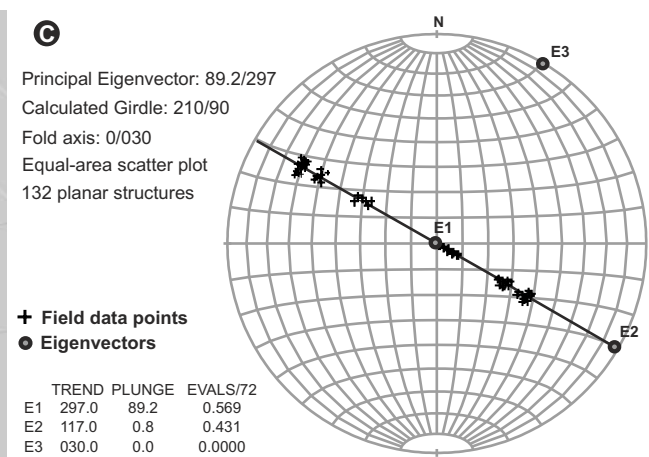
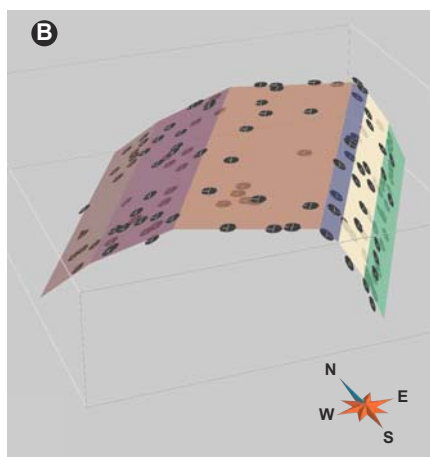
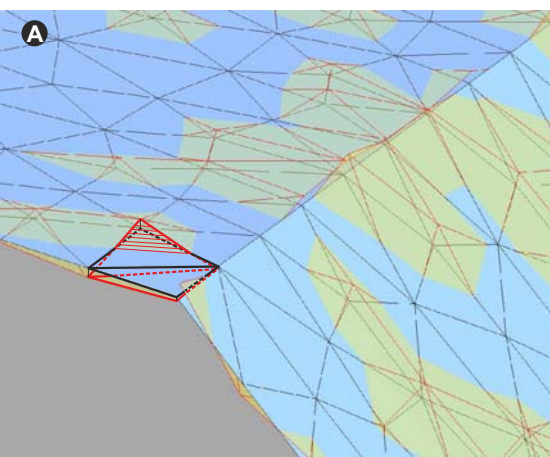
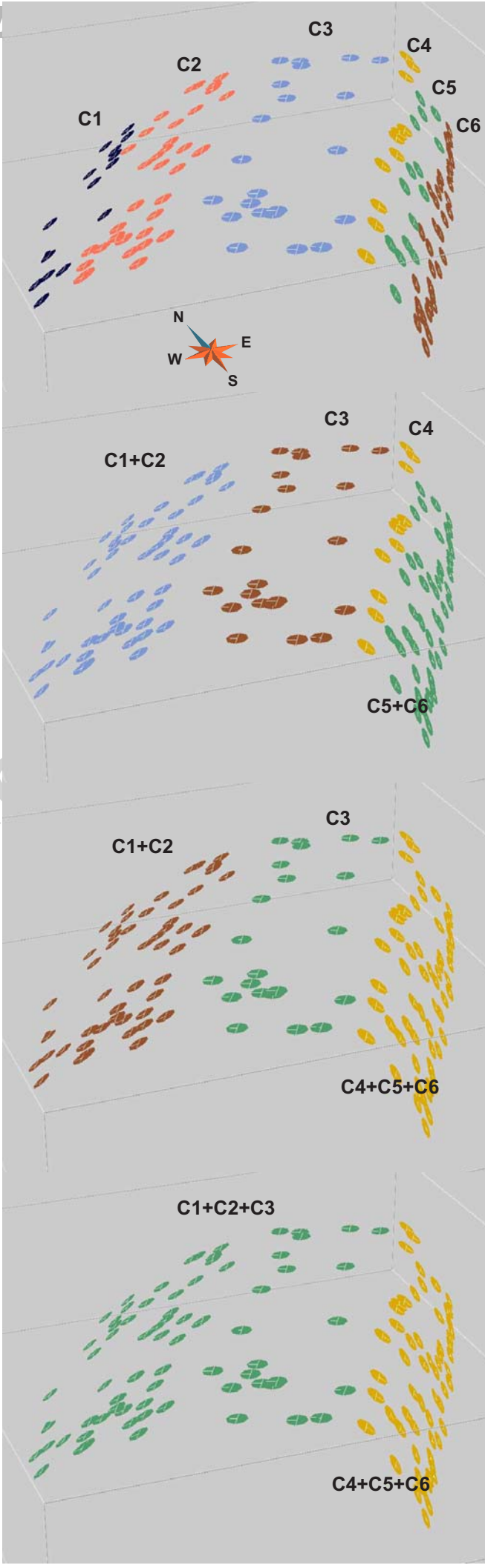
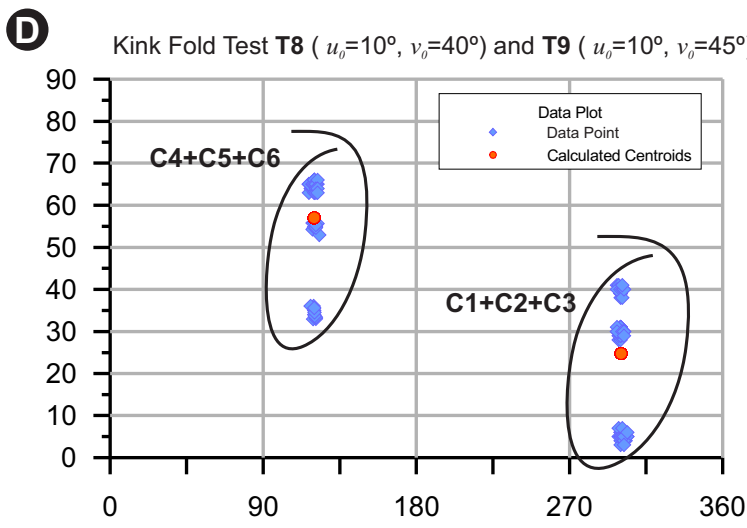
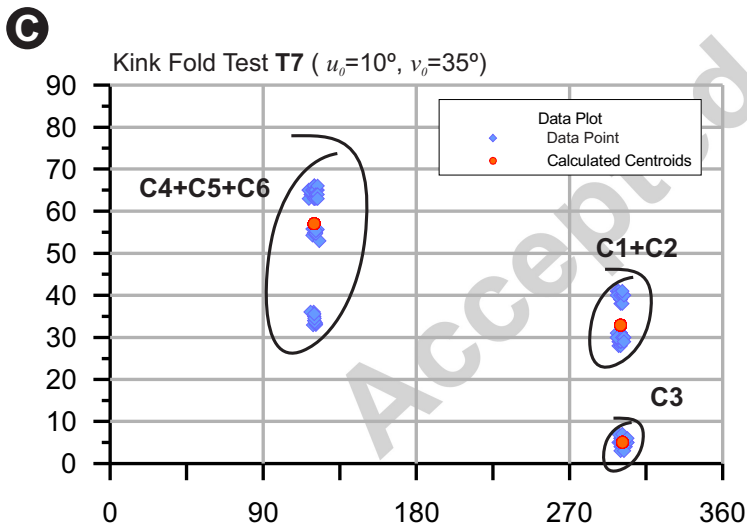
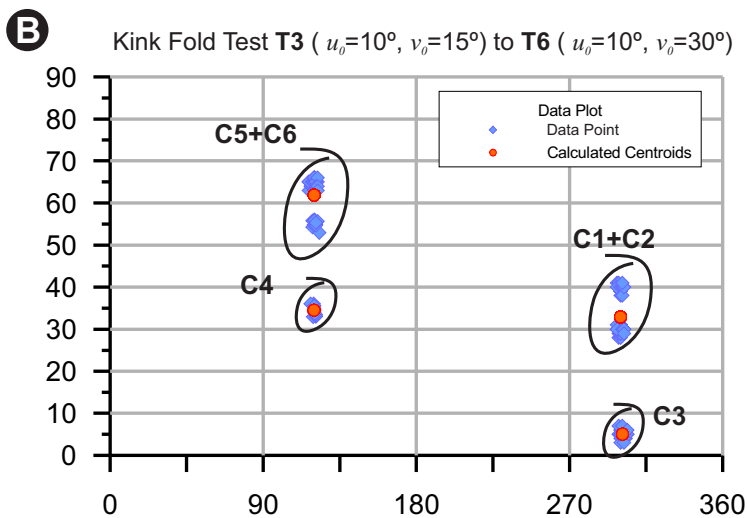
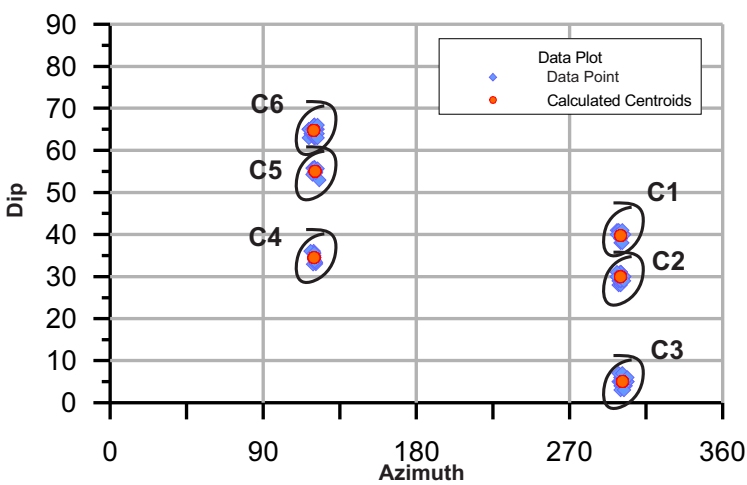
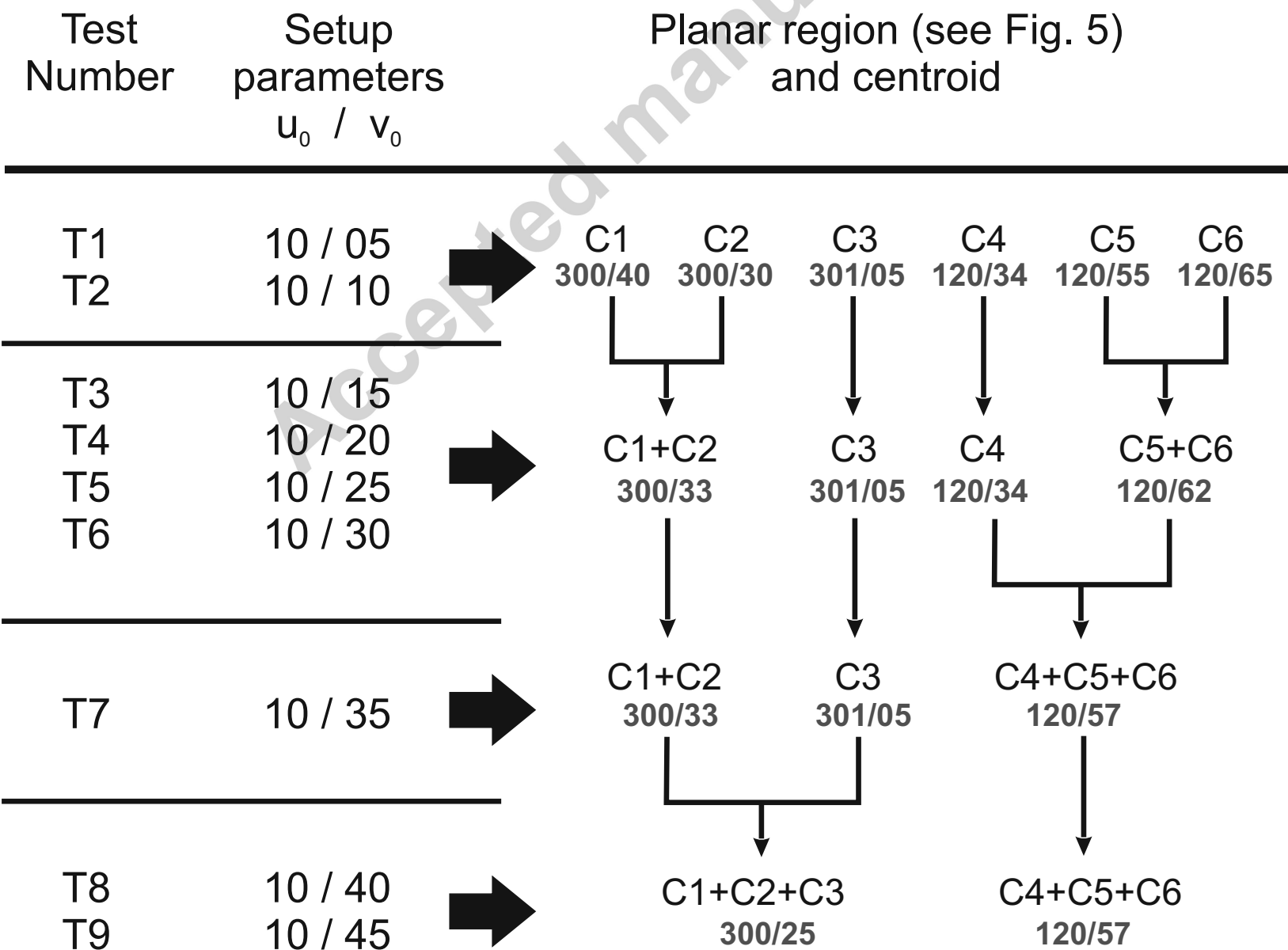
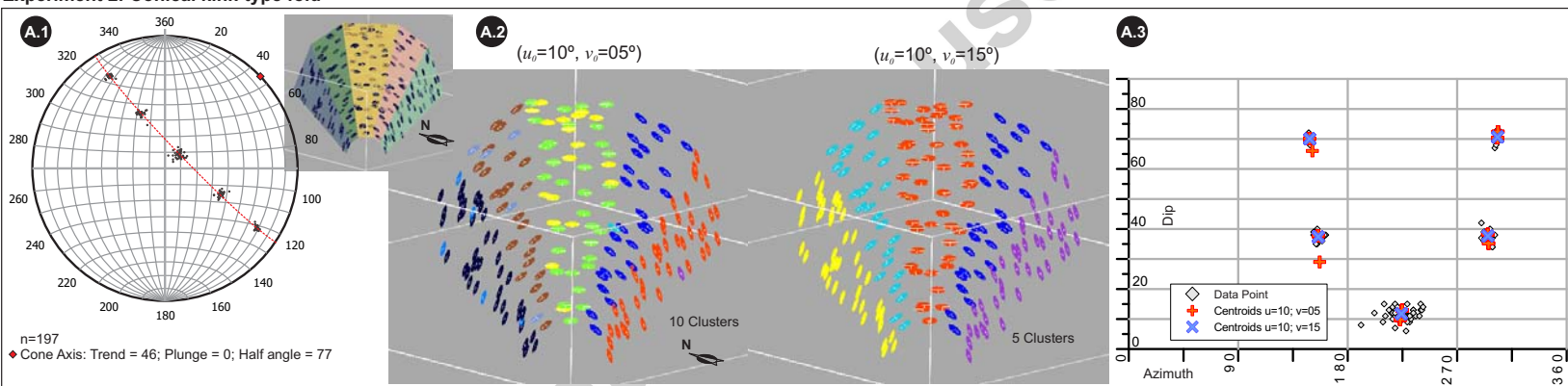


Figure 5 Kink Fold Test **T1** ($u_0=10^\circ, v_0=5^\circ$) and **T2** ($u_0=10^\circ, v_0=10^\circ$)

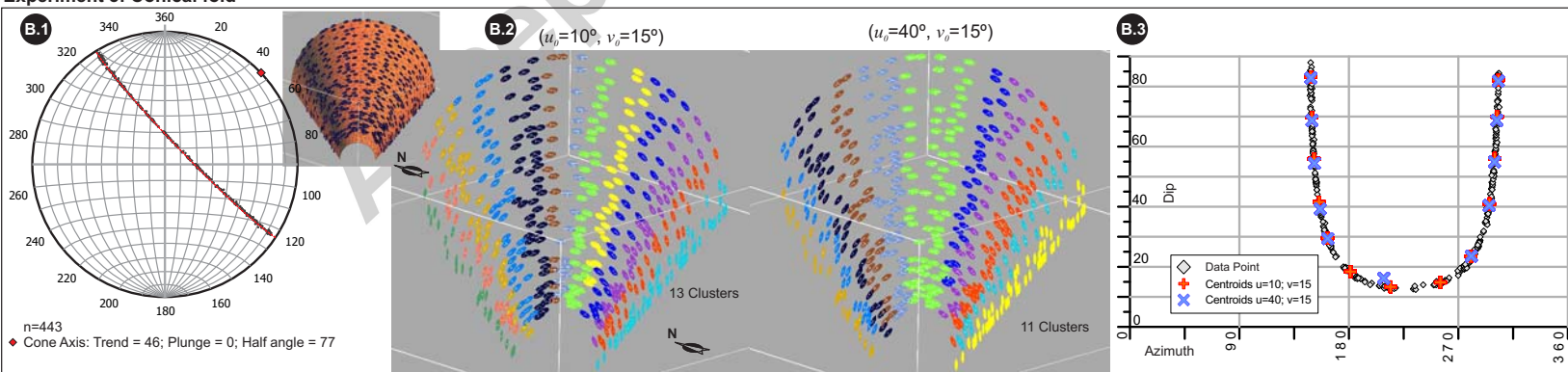




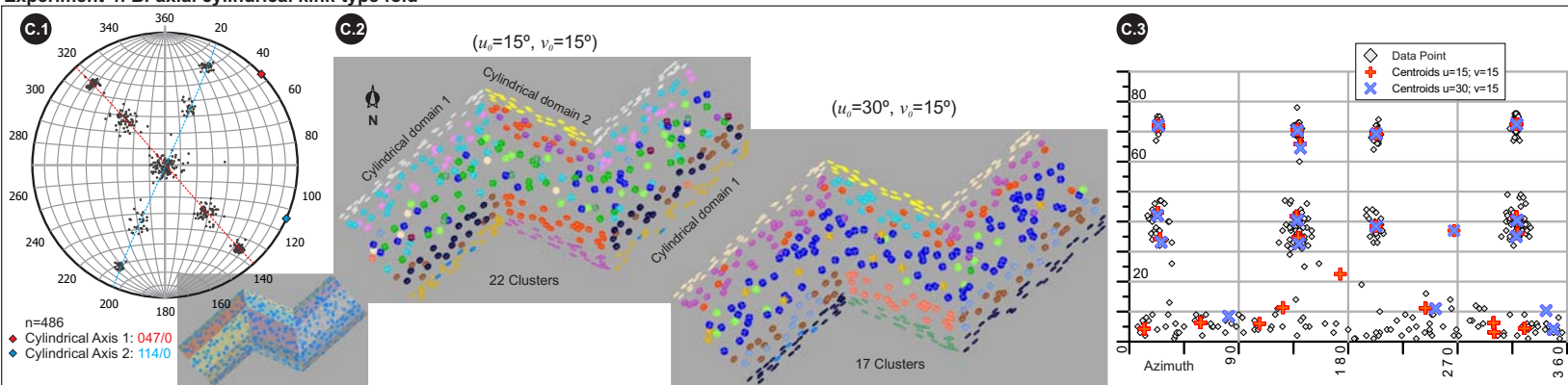
Experiment 2: Conical kink-type fold



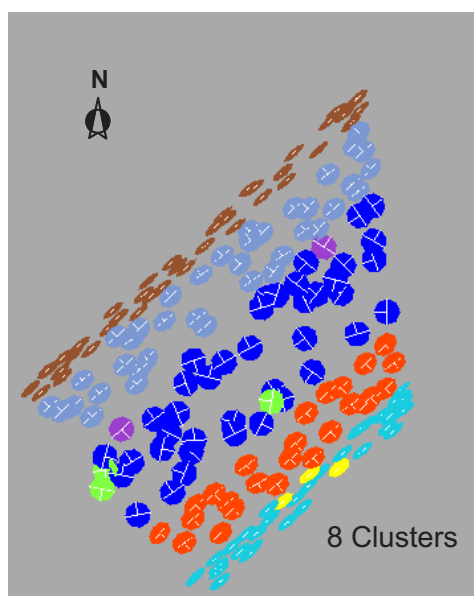
Experiment 3: Conical fold



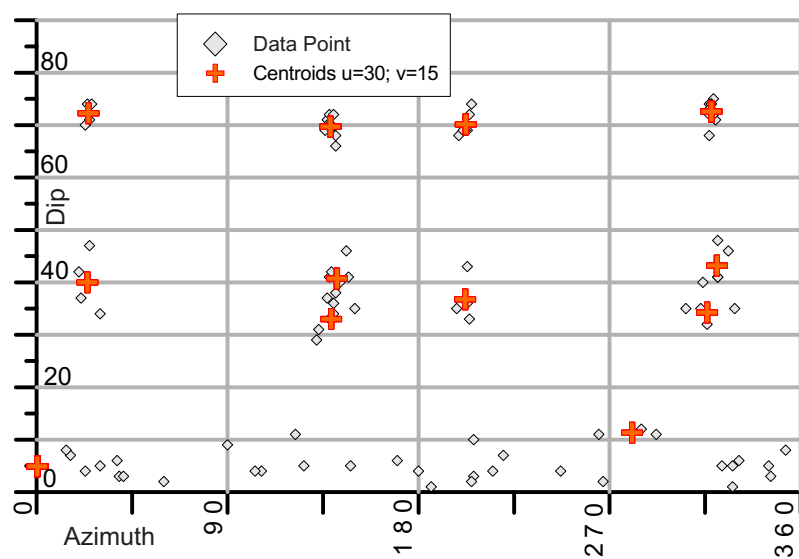
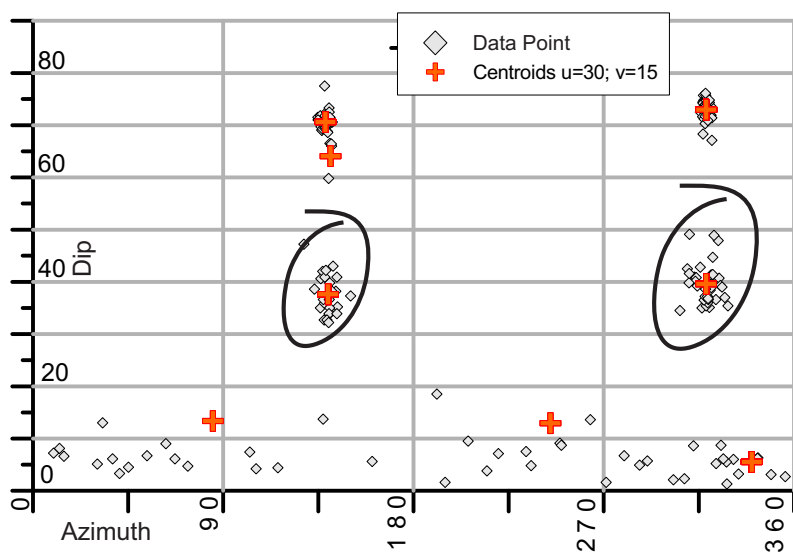
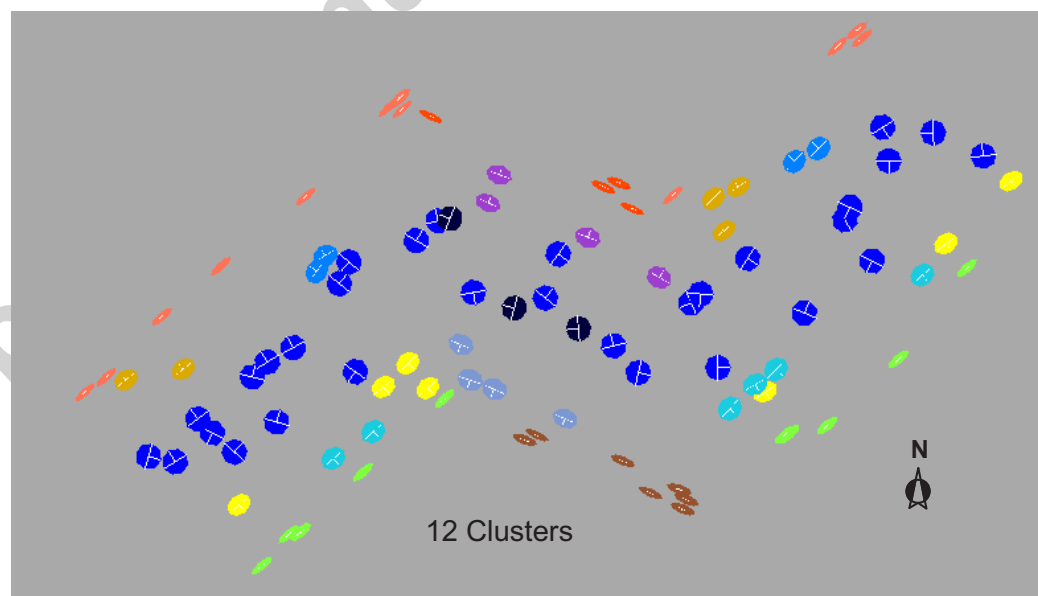
Experiment 4: Bi-axial cylindrical kink-type fold

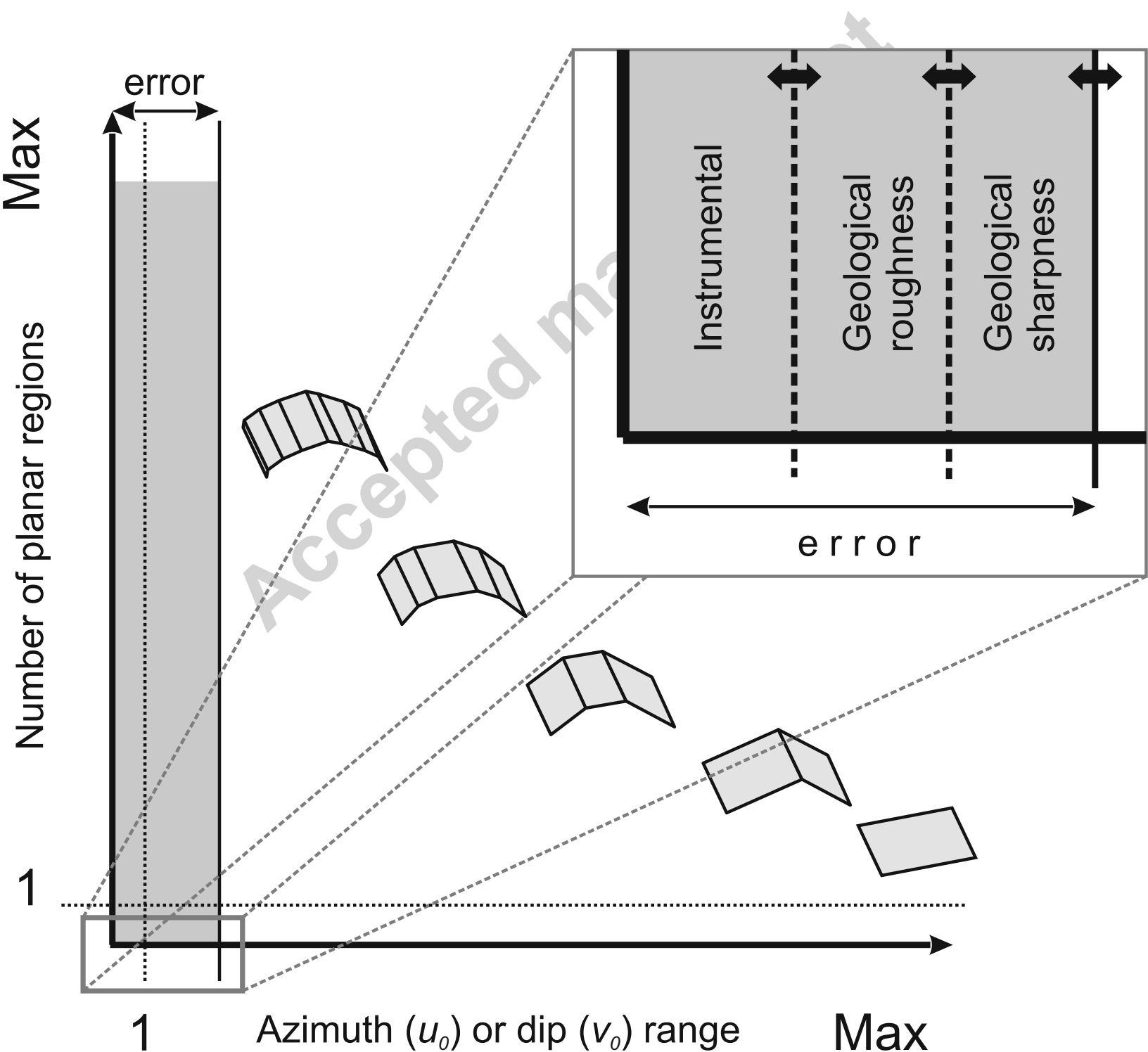


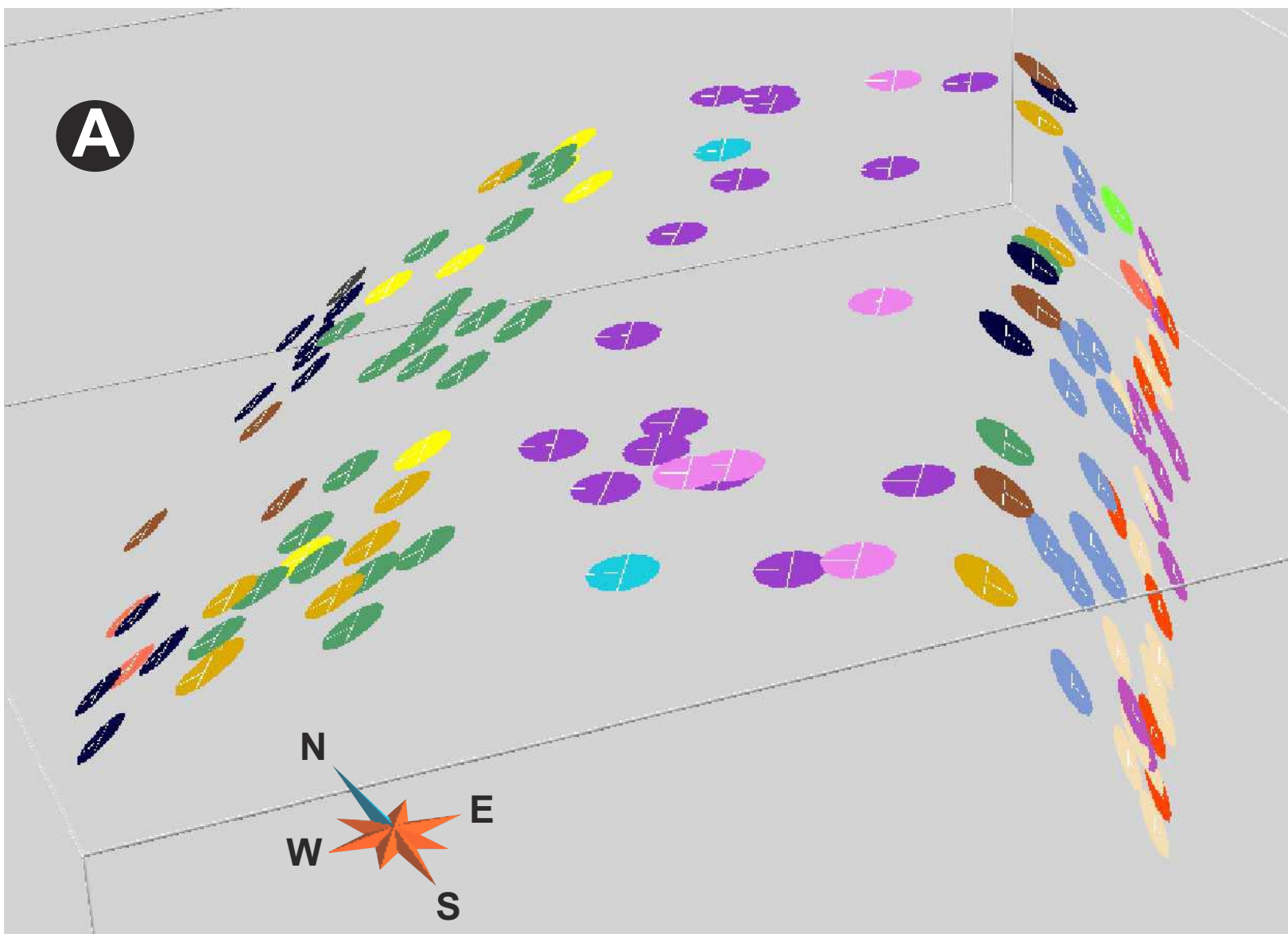
A Experiment 5:
Cylindrical kink-type fold subset
($u_0=30^\circ$, $v_0=15^\circ$)



B Experiment 6:
Bi-axial cylindrical kink-type fold subset
($u_0=30^\circ$, $v_0=15^\circ$)







B

Setup
parameters
 u_0 / v_0

Number of
Planar Domains

10 / 1

21

10 / 0.5

29

10 / 0.1

39