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1 **Localisation of normal faults in multilayer sequences**

2
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7
8 **Abstract**

9 Existing conceptual growth models for faults in layered sequences suggest that faults
10 first localise in strong, and brittle, layers and are later linked in weak, and ductile,
11 layers. We use the Discrete Element Method (DEM) for modelling the growth of a
12 normal fault in a brittle/ductile multilayer sequence. The modelling reveals that faults
13 in brittle/ductile sequences at low confining pressure and high strength contrast
14 localise first as Mode I fractures in the brittle layers. Low amplitude monoclinial
15 folding prior to failure is accommodated by ductile flow in the weak layers. The
16 initially vertically segmented fault arrays are later linked via shallow dipping faults in
17 the weak layers. Faults localise, therefore, as geometrically and kinematically
18 coherent arrays of fault segments in which abandoned fault tips or splays are a
19 product of the strain localisation process and do not necessarily indicate linkage of
20 initially isolated faults. The modelling suggests that fault tip lines in layered
21 sequences are more advanced in the strong layers compared to weak layers, where the
22 difference in propagation distance is most likely related to strength and/or ductility

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23 contrast. Layer dependent variations in fault propagation rates generate fringed rather
24 than smooth fault tip lines in multilayers.

25

26 *Keywords:* Discrete Element Method; fault growth; fault refraction; fault tip line;

27 Mohr circles; stress and strain paths;

28

29 **1 Introduction**

30 There are a variety of conceptual models for the growth of faults in mechanically
31 layered (brittle/ductile) sequences, all of which acknowledge that faults commonly
32 show lithologically controlled dip changes on cross-sections, with steeper fault dips in
33 strong layers and shallower dips in weaker layers (Fig. 1). These dip changes are
34 attributed to a variety of mechanisms (Ferrill and Morris, 2003 and references
35 therein): (i) post-faulting differential compaction, (ii) active faulting, with slip along
36 layers or intersecting faults, (iii) linkage of an originally vertically-segmented fault
37 and (iv) fault initiation with dip controlled by rock properties and effective stresses.
38 Two of these mechanisms (iii and iv), which are not mutually exclusive, underpin the
39 most popular models for the growth of faults within layered sequences. For
40 mechanism (iii) faults first localise in the strong layers and are later linked via faults
41 in the weak layers (Peacock and Sanderson, 1992; Eisenstadt and De Paor, 1987;
42 Childs et al., 1996; Crider and Peacock, 2004). In this case, fault localisation and dips
43 within the strong layers are controlled by rock properties and deformation conditions,
44 and therefore by the failure mode and/or failure angles, while dips within the weak
45 layers are a consequence of segment linkage. An alternative model (iv) suggests that
46 localisation and associated dip changes do not develop in association with fault
47 segmentation and are entirely controlled by the failure mode and failure angles of the
48 faulted weak and strong layers. Distinguishing between these models on observational
49 or theoretical grounds is not, however, always straightforward.

50 Ferrill and Morris (2003) describe small-scale faults exhibiting lithologically
51 controlled dip variations. These authors consider two mechanisms of formation for the
52 fault geometries they observe, these are, fault localisation first occurs within the
53 strong layers (Fig. 2b) and fault localisation first occurs within the weak layers (Fig.

54 2c). In both cases fault dips are determined by the rheological properties of the layers
55 with steep dips in the strong layers and relatively shallow dips in the weak layers. The
56 faults studied by Ferrill and Morris (2003) do not have geometrical features which
57 might indicate whether they initiated in the strong or weak layers, e.g. abandoned tips
58 or splays. Other workers have described faults with lithologically controlled dip
59 variations which, from field relations, can be demonstrated to have formed by linkage
60 of segments which formed within the strong layers (e.g. Peacock and Zhang, 1993,
61 Childs et al., 1996). The absence of discriminating traits of segmentation, may support
62 the application of a model in which the faults were not, in fact, segmented in their
63 early stages of growth, but formed by refraction across bedding planes during
64 progressive forward tip-line propagation (Fig. 2d).

65 Although both linkage and forward propagation models (Fig. 2) provide a
66 plausible rationale for field observations that can be related to failure criteria, they
67 otherwise lack a mechanical basis. Mechanical analyses using failure criteria (e.g.
68 Coulomb-Mohr, Griffith) can provide useful insights into the orientation of principal
69 stresses and consequently faults, but do not allow definition of the relative timing of
70 failure and localisation in a mechanical multilayer (Mandl, 2000).

71 Since observational data and theoretical grounds do not provide a definitive
72 answer to questions relating to the localisation of faults within multilayers, we use a
73 numerical modelling approach which is capable of localising faults within multilayer
74 sequences. The aim of this paper is to provide a mechanical basis for the localisation
75 and linkage of normal faults in a layered sequence using the Discrete Element Method
76 (DEM). DEM has recently been used for modelling the formation of accretionary
77 wedges (Burbidge and Braun, 2002), fault-propagation folds (Finch et al., 2003 and
78 2004), out-of-plane fault propagation (Strayer and Suppe, 2003) and the interaction of

79 two overlapping faults (Imber et al., 2004). The method is capable of modelling
80 failure and localisation without the necessity to define constitutive equations, as is the
81 case for the more commonly used continuum methods. It is therefore the ideal tool for
82 addressing questions relating to fault localisation in multilayered brittle/ductile
83 sequences. As is described later, our models comprise brittle materials that deform by
84 elastic deformation followed by fracturing and ultimately failure at peak strength,
85 whilst our ductile material is frictional-plastic throughout deformation, displaying an
86 inelastic deformation response without fracturing; these materials lead to macroscopic
87 deformations that are discontinuous and continuous respectively. The results of the
88 modelling support the notion that vertically segmented fault arrays initially develop in
89 the strong, and brittle, layers and are later linked by shallower dipping faults in the
90 weak, and ductile, layers.

91

92 **2 Methods**

93 2.1 *Principles of DEM*

94 The Discrete Element Method is a broad class of methods for modelling the finite
95 displacements and rotations of discrete bodies (Cundall and Hart, 1992). DEM can be
96 implemented in two and three dimensions. We use a 2D approach with circular
97 particles as introduced by Cundall and Strack (1979) and implemented in
98 commercially available software (*PFC-2D*, Itasca Consulting Group, 1999). Particles
99 are treated as rigid discs and are allowed to overlap at particle-particle and particle-
100 wall contacts. Walls are rigid boundaries of arbitrary shape, to which constant
101 velocity or constant stress conditions can be applied. The amount of overlap at each
102 contact is small compared to particle size and the contact normal force is linearly
103 related to the amount of overlap. If the contact shear force exceeds a critical value,

104 which is determined by a contact friction coefficient, slip occurs at the contact.
105 Particles can be bonded together with linear elastic cement (parallel bond model,
106 Itasca Consulting Group, 1999; Potyondy and Cundall, 2004) and if the critical tensile
107 or shear stress (which is typically normally distributed in a bonded model) at a bonded
108 contact is exceeded the bond breaks.

109 For a more detailed description of this numerical method the reader is
110 referred to Cundall and Hart (1992), Hazzard et al. (2000), Potyondy and Cundall
111 (2004) and references therein.

112

113 2.2 *Model material calibration*

114 In contrast with continuum methods, where the rheology of the model material is
115 defined using constitutive laws, the macroscopic response of the (bonded) particle
116 assemblage in DEM models has to be calibrated using a numerical laboratory. The
117 microproperties (particle size and size distribution, particle and bond stiffness, contact
118 friction, bond strength) are adjusted, mainly by trial and error, to obtain the desired
119 model macroscopic response calibrated to laboratory rock deformation data. The
120 resulting microproperties do not replicate true grain-scale physics because the model
121 particles are orders of magnitude larger than the grains of the equivalent rock and
122 each particle therefore represents a small volume of rock. Although our approach did
123 not attempt to exactly reproduce the rheology of a particular rock based on
124 experimental data, the macroscopic properties of our model materials reproduce the
125 general rheological behaviour of a strong, brittle material and a weak, ductile one.

126 The particles in this study have a uniform size distribution with r_{\max} and r_{\min}
127 of 62.50mm and 31.25mm, respectively. The rheology of a strong material, consisting
128 of bonded particles, and a weak material, consisting of non-bonded particles, was

129 investigated. The bonded particles have normal and shear contact/bond stiffnesses of
130 50GPa and 16.7GPa, respectively, a contact friction coefficient of 1.0 and normally
131 distributed tensile and shear bond strengths with a mean of 250MPa and 125MPa and
132 coefficients of variation of 1/12 and 1/6, respectively. The bond strength distributions
133 have cut-offs of plus/minus two standard deviations and the width of each bond is half
134 the radius of the smaller of the two bonded particles. The non-bonded particles have
135 the same particle size and size distribution as the bonded material, a normal and shear
136 contact stiffness of 50GPa and 16.7GPa, respectively, and a contact friction
137 coefficient of 0.5.

138 The strength of bonded materials is sample size dependent (strength
139 decreases with increasing sample size; Potyondy and Cundall, 2004), thus proper
140 calibration requires tests on samples at a scale appropriate to the model. In our
141 multilayer modelling, the basic mechanical unit is one bed. Therefore the rheology of
142 both the bonded and non-bonded material was investigated using calibration sample
143 widths equal to the thickness of the strong layers in the multilayer, i.e. 1m (see
144 below).

145 The rheology of the non-bonded material was investigated using confined
146 (25MPa) biaxial compression tests on samples that are 1m wide and 2m high. Since
147 the material is cohesionless and exhibits no (bulk) elasticity the only bulk property
148 that was calculated for each test ($N = 30$) is the friction coefficient, which can be
149 easily obtained for straight failure envelopes.

150 The rheology of the bonded material was investigated using unconfined
151 biaxial compression tests on samples that are 1m wide and 2m high. These tests ($N =$
152 30) were used for calculating the bulk elastic properties (Young's modulus, Poisson's
153 ratio) and provided the unconfined compressive strength. Additionally direct tension

154 tests on dog-bone shaped samples ($N = 196$) with a central thickness of 1m were
155 performed at various confining pressures in order to define the failure envelope in the
156 tensile stress field.

157 Although calibration tests on 1m wide samples provide the bulk rheological
158 properties and their variability at the scale of the multilayer model, they do not give
159 insights into strain distribution (e.g. localisation) within the sample due to their poor
160 resolution (*ca* 10 particles wide). To examine localisation behaviour in our model
161 materials nine biaxial tests were performed on samples that are 5m wide and 10m
162 high and contain over 6000 particles.

163

164 2.3 *Multilayer faulting model boundary conditions*

165 The multilayer model used is 15m wide, 13m high and is comprised of >23,400
166 particles (Fig. 3a). The model is composed of four 1m thick strong (bonded particles)
167 and four 1.5m thick weak (non-bonded particles) layers. The top 3m of the model
168 comprises a layer of non-bonded particles. The primary function of this top layer is
169 model confinement, which is achieved by applying a force equivalent to a lithostatic
170 stress of approximately 23MPa (*ca* 1km burial depth) to particles at the surface of the
171 model. The sides and base of the model are defined by two rigid L-shaped walls
172 which meet at a predefined 60° dipping fault at the base of the model. The L-shaped
173 hanging wall is moved with constant velocity parallel to the predefined fault; this pre-
174 conditioning ensures the formation of one fault, rather than several faults. The model
175 is saved in 1cm throw increments and the final throw is 10cm; models with throws
176 beyond the point of localisation (*ca* 10cm) will be published elsewhere. With respect
177 to the ideal elliptical fault surface shown in Fig. 3b, the model is located in the plane
178 of no lateral propagation along a chord through the point of maximum displacement.

179

180 2.4 *Stress and strain in discontinua*

181 Stress and strain are continuum concepts, whereas our model material is comprised of
182 discrete particles and is therefore a discontinuum (compressive stress positive and σ_I
183 $> \sigma_{II} > \sigma_{III}$). Various methods for homogenising DEM models to allow comparison
184 with continuum mechanics solutions have been proposed and successfully
185 implemented (e.g. O'Sullivan et al., 2003). The stress tensor can be obtained for each
186 particle in our models, but the state of stress at this point is meaningless on a
187 macroscale, i.e. on the scale of the layers. To homogenise particle stresses the average
188 stress tensor is calculated for circular regions (Potyondy and Cundall, 2004).

189 The deformation tensor \mathbf{D} , which is sometimes called the positions gradient
190 tensor (see Appendix A), can be obtained for small and large strains using the least-
191 squares method described in Oda and Iwashita (2000). For each circular region
192 (diameter depends on the scale of interest) the particle closest to the centre is found
193 and the relative displacements of particles surrounding this particle are calculated in
194 order to remove the translational component of deformation. Once this translation has
195 been removed the best-fit displacement gradient tensor can be calculated, enabling the
196 deformation tensor \mathbf{D} and the Lagrangian strain tensor \mathbf{E} to be obtained.

197 For the maximum shear strain contour diagrams shown (e.g. Fig. 4e and f,
198 Fig. 6) the diameter of the circular homogenisation area is 0.3m, contains, on average,
199 eight particles and the best-fit displacement gradient tensor is obtained for each
200 particle. Since the averaging region is a small proportion of the model dimensions,
201 contours of (maximum shear) strain are typically quite irregular. We present both
202 finite and incremental strain contours to illustrate fault evolution. Incremental strains
203 are calculated in 1cm throw intervals, where for each particle the accumulated

204 displacement of the previous stage is subtracted. The best-fit deformation tensor for
205 each 1cm throw increment can then be obtained for each particle using the same
206 method described above.

207 For the definition of the stress and strain paths at selected locations within
208 our model (Fig. 8) we use 1m diameter homogenisation areas, containing on average
209 92 particles, to minimize noise. Strain paths are represented using Mohr circles for the
210 deformation tensor, which are briefly reviewed in Appendix A.

211

212 **3 Results**

213 3.1 *Macroproperties of model material*

214 Stress vs. axial strain (Fig. 4a and b) and volumetric strain (strictly speaking area
215 change in a 2D model) vs. axial strain (Fig. 4c and d) curves for the strong and weak
216 model material are shown in Fig. 4 (high resolution models, 5m wide and 10m high).
217 Additionally maximum shear strain contour plots for selected biaxial test samples are
218 shown (Fig. 4e and f) in order to illustrate strain localisation. The strong material
219 exhibits elasticity and compaction prior to failure (Fig. 4a). The axial strain at failure
220 and the differential stress at failure increase with increasing confining pressure (Fig.
221 4a). The amount of strain softening decreases with increasing confining pressure, i.e.
222 the material becomes more ductile. The weak material exhibits steady-state flow after
223 a non-linear increase in differential stress (Fig. 4b). The steady-state stress increases
224 with increasing confining pressure. The lack of strain softening in the weak material is
225 probably due to the use of rigid platens as lateral boundaries, which do not allow the
226 formation of a single through-going shear zone (O'Sullivan pers. comm., 2004). A
227 comparison of the volumetric strain curves for the strong and weak material (Figs. 4c
228 and d) reveals that at low confining pressures (e.g. 25MPa, see also max. shear strain

229 contour plots, Figs. 4e and f) the weak material dilates and localises earlier than the
230 strong material. However, from these figures it is clear that the strong material
231 localises strain better because it exhibits greater strain softening.

232 Young's modulus and Poisson's ratio (assuming plane strain, Potyondy and
233 Cundall, 2004) were obtained for the unconfined biaxial tests (sample width 1m, $N =$
234 30) and determined at half the axial strain to failure and are 21.8 ± 1.6 GPa and $0.29 \pm$
235 0.06, respectively. Principal stress diagrams with best-fit failure envelopes are shown
236 in Fig. 5. For the strong material a Coulomb-Mohr criterion with tension cut-off (Paul,
237 1961) was fitted using the results of direct tension tests on dog-bone shaped samples.
238 The best-fit parameters with curves representing probabilities that data points lie on
239 the left hand side of the failure envelope are plotted in Fig. 5 and reveal that the
240 unconfined compressive strength, cohesion and friction coefficient are typical of those
241 for strong sedimentary rocks (e.g. Hoek and Brown, 1997; Tsiambaos and
242 Sabatakakis, 2004). However, the ratio of unconfined compressive strength to tensile
243 strength is low (3.5) compared to natural rocks (e.g. 9–17, table 6.15.1 in Jaeger and
244 Cook, 1976). These low ratios are typical for DEM models using smooth, circular
245 particles (Fakhimi, 2004) and can be improved using either irregular shaped particles
246 (clumps), by introducing a bending resistance between chains of bonded particles
247 (Cundall pers. comm., 2004) or by increasing sample resolution (table 3 in Potyondy
248 and Cundall, 2004). For the purpose of this article in which we examine fault
249 localisation within a brittle/ductile sequence, absolute strength values are subordinate
250 with strength contrast and rheology the main controlling factors. For the non-bonded
251 material the average friction coefficient was calculated from the confined biaxial tests
252 as 0.47 ± 0.05 (standard deviation). The Coulomb-Mohr criterion is plotted using the
253 average friction coefficient and no cohesion (Fig. 5).

254 In summary, material properties and rheology of the strong layers are
255 comparable with those of strong sedimentary rocks (e.g. Hoek and Brown, 1997;
256 Tsiambaos and Sabatakakis, 2004), whilst the weak layers have no tensile strength
257 and are comparable to some shales (e.g. Petley, 1999).

258

259 3.2 *Fault growth and geometry in a multilayer sequence*

260 Figure 6 shows the propagation of a fault through a multilayer model at throw (t)
261 increments of 1cm. The stages of fault evolution are illustrated with contours of
262 incremental maximum shear strain for each stage. Although the total 10cm offset is
263 not visible from the layer interfaces, fault development can be examined from the
264 changing pattern of low incremental strains. Figure 6 is complemented by the profiles
265 of strain and rotation for layer E at 2cm throw increments (Fig.7), which were
266 obtained using 1m wide circular homogenisation regions with a spacing of 10cm.

267 At low displacements ($< 3\text{cm}$) diffuse zones of deformation develop on either
268 side of the lowest strong layer (G). Up to throws of 3cm, formation of a low-
269 amplitude precursory fold within this strong layer is accommodated by flow in the
270 underlying and overlying weak layers. At a throw of 4cm, the lowest strong layer (G)
271 fails in tension (Mode I fracture) and subsequent strain is concentrated on this fault.
272 At throws of 5cm to 7cm, flow in the weak layers accommodates folding of the
273 second strong layer (E) until it fails in tension arising from outer-arc extension
274 associated with monoclinial folding; folding is highlight by the rotational plateaux
275 shown in Fig.7. Flow in the weak layers is principally accommodated within diffuse
276 zones that are located in the hanging wall of the incipient fault and have an overall
277 antithetic shear sense (see below). These antithetic shear zones intersect the tops of
278 the strong layers at the point of greatest outer arc extension associated with

279 monoclinical folding. At a throw of 8cm two additional Mode I fractures have formed,
280 one in the topmost layer (A), collinear with the array of underlying Mode I fractures,
281 and another one in the hanging wall of the lowest layer (G). The latter is located on
282 the hanging wall hinge of the monoclinical flexure of the lowermost strong layer and
283 propagates from bottom to top, a direction that is again consistent with outer arc
284 extension. At this stage one of the strong layers (C) is still intact, even though it is
285 overlain and underlain by strong layers containing an approximately collinear array of
286 Mode I fractures, demonstrating that the failure of layers within a multilayer does not
287 necessarily occur in forward sequence. At a throw of 9cm the fault has cut through all
288 of the strong layers within the sequence and although it begins to localise within the
289 weak layers, it has yet to do so in the central weak layer. This anomaly arises due to
290 the localisation of a second Mode I fracture in the second lowest strong layer (E). This
291 new fracture formed in the hanging wall side of the earlier fracture, which became
292 inactive over the 8 - 9cm interval but became active again between 9 - 10cm throw. At
293 10cm throw a continuous, through-going fault is established. This fault has a
294 'staircase' geometry, in which vertical faults within the strong layers are linked by
295 approximately 50° dipping faults in the weak layers, producing an average dip of *ca*
296 60°. Although individual fault segments first develop within strong layers and do not
297 progress simply from bottom to top of the model, the final geometry is relatively
298 simple and coherent. This coherence suggests that the deformation of both strong and
299 weak layers throughout the model is strongly coupled, details of which are
300 investigated below.

301

302 3.3 *Stress and strain paths*

303 The centre diagram in Fig. 8 shows the model in Fig. 6 at the final throw of 10cm
304 contoured for maximum finite shear strain (contour interval is 0.01). Strain and stress
305 paths were determined at 12 selected locations (Fig. 8). In each circular region of 1m
306 diameter the average stress tensor and displacement gradient tensor were obtained at
307 1cm throw intervals. For the strong layers, six locations of Mode I fracturing were
308 analysed, four along the eventual through-going fault and two hanging wall splays. In
309 the weak layers, four regions were examined between the main Mode I fractures in the
310 strong layers and along the eventual through-going fault, and two regions were
311 selected within the low-angle antithetic shear zones in the hanging wall of the
312 eventual through-going fault. The strain paths are shown in Fig. 8 using Mohr circles
313 for the deformation tensor (see Appendix A for a brief review). Rotations and
314 stretches are easily read off these diagrams (see Fig. A-2 for ideal deformation paths)
315 and large volumetric strains can be simply calculated by the product of the principal
316 stretches. However, the volumetric strains and rotational components of strain in this
317 model were initially small and are therefore shown separately in Fig. 9 for each
318 locality. Stress paths are shown in principal stress diagrams in Fig. 10, in which the
319 experimental derived failure envelopes for the strong and weak material (Fig. 5) are
320 plotted.

321 The strain and stress paths of the 12 locations identified in Fig. 8 are
322 described in four groups sharing similar evolutionary paths. Each of these groups
323 represents a key kinematic element of the localisation of the fault within the modelled
324 multilayer. For simplicity the groups are referred to in geometric terms relative to the
325 eventual through-going fault and depending on whether they occur within strong or
326 weak layers. They are each described in the general order in which they develop: (i)

327 antithetic shear zones - weak layers, (ii) synthetic faults, strong layers, (iii) synthetic
328 faults – weak layers, (iv) hanging wall splays – strong layers; whilst the structures i
329 and iv represent accommodation features associated with fault displacement, the
330 synthetic faults (ii and iii) eventually become the through-going fault. Though the
331 emphasis is on describing the basic deformation paths for each element, we also
332 highlight the coupling and inter-relationships between them. The location of each
333 locality is shown in Fig. 8 (with locality names ranging from A through to H
334 according to the layer), and individual strain and stress paths for each of these
335 locations are shown in Figs. 8, 9 and 10.

336 (i) Antithetic shear zones – weak layers:

337 The two locations (D2 and F2) straddling antithetic shear zones in weak layers show
338 similar strain/stress paths, though the zone closer to the base of the model and the
339 future main fault (F2) shows, as expected, the larger volumetric strain and finite
340 strain. These zones are dilational (Fig. 9b) with generally counter-clockwise (CCW)
341 shearing (positive rotation in Fig. 8 and 9d), a dominant pure shear component (Fig.
342 8) and link downwards into eventual Mode I fractures which form the main fault
343 within the strong layers (Fig. 6). Their formation is evidently related to monoclinial
344 folding of the intervening strong layers because they link the eventual Mode I
345 fractures arising from outer arc folding of underlying strong layers with the
346 complementary monoclinial hinge on the base of overlying strong layers (Fig. 7). After
347 the first throw increment (1cm) the weak material at both locations is in its critical
348 stress state (Fig. 10b) and thereafter shows an almost linear increase in volumetric
349 strain with throw (Fig. 9b). The continued growth of these antithetic shears suggests
350 that flexuring within the hanging wall of the eventual main fault continues beyond the
351 formation of Mode I fractures within the strong layers (Fig. 7), a feature which is

352 ascribed to the irregularity of the trace of the eventual through-going main fault (see
353 below). A temporary levelling off of volumetric strain at one location (D2, Fig. 9b) is
354 attributed to the short-term cessation of extension across the Mode I fracture in the
355 second lowest strong layer (location E1).

356 (ii) Synthetic faults – strong layers:

357 Four locations (A, C, E1 and G1; Fig. 8) straddle the trace of the main fault within the
358 strong layers and show similar stress/strain paths, though timing differs from one
359 location to another. Initially the deformation at each location is characterised by
360 clockwise (CW) rotation (negative values in Fig. 9c) accompanied by approximately
361 linear increase in volumetric strain (Fig. 9a) and progressive increase in σ_I and
362 decrease in σ_{III} (Fig. 10a). These deformations are consistent with monoclinial folding
363 prior to fault localisation (Fig. 7). Tensile failure, i.e. Mode I fracture, of each strong
364 layer is marked by a rapid increase in the local volumetric strain (Fig. 9a), a slight
365 increase in rate of rotation (Fig. 9c) and, generally, by a corresponding stress release
366 (increase in σ_{III} , Fig. 10a). The rapid volumetric strain changes and associated Mode I
367 fracture formation do not, however, migrate progressively up the model with time.
368 From the base of the model Mode I fracturing starts in the strong layers at 3cm throw
369 (G1), *ca* 4.5cm (E1), 8cm (C) and 7cm (A), respectively. After Mode I fracturing,
370 most locations are characterised by simple extension (Fig. 8) with increasing
371 dilational CW shear (Fig. 9a and c), arising from pull-apart formation. A temporary
372 cessation of displacement on the second lowest layer (at E1) is marked by a gradual
373 increase in CW rotation (Fig. 9c) and a decrease in both σ_I and σ_{III} (Fig. 10a), with
374 approximately constant volumetric strain (Fig. 9a). This is due to the formation of a
375 Mode I fracture in the hanging wall of the main fault, which is active in the last two
376 throw increments shown (see hanging wall splay – strong layer, location E2).

377 (iii) Synthetic faults – weak layers:

378 Four locations (B, D1, F1 and H) straddle what is to become the main fault within the
379 weak layers. One of these (location H) reaches an advanced stage very early because
380 it is adjacent to the pre-defined fault and therefore attains high strains at low throws,
381 immediately reaching the critical stress state of the weak material (Fig. 10b) and
382 thereafter showing approximately linear increases in volumetric strain with throw
383 (Fig. 9b). The rotational component at this location shows a dramatic increase after a
384 throw of 4cm (Fig. 9d), which coincides with the formation of the first Mode I
385 fracture (location G1). In contrast the other locations (B, D1 and F1) are characterised
386 by early stage CW rotations (Fig. 9d) with variable degrees of compaction (Fig. 9b),
387 which are usually accompanied by increases in σ_I and little change in σ_{III} (Fig. 10b).
388 Later stage decreases in both σ_I and σ_{III} (Fig. 10b) together with increases in
389 volumetric strain (Fig. 9b) are associated with dilational CW shearing with a
390 dominant simple shear component (Fig. 8). Rotation associated with monoclinial
391 flexure occurs in each weak layer from the onset but increases abruptly at a throw of
392 8cm (Fig. 9d) when the final strong layer (C) is broken and elevated shear strains
393 occur along the entire fault trace (Fig. 6). This late stage deformation reflects fault
394 linkage and the relative shallow dip of the linking faults within the weak layers. At
395 this stage the weak material is in a critical stress state (Fig. 10b) and thereafter shows
396 an approximately linear increase in volumetric strain with throw (Fig. 9b). Again the
397 overstep generation is not progressive with linkages occurring at *ca* 4cm throw in the
398 lower part of the model (at F1), at *ca* 8cm towards the top of the model (at B) and at
399 *ca* 10cm towards the middle of the model (at D1). Though the deformation paths of
400 each of the locations are similar, slight differences may offer some clues to the
401 localisation process. The retarded localisation of a through-going fault at D1 is

402 associated with the relatively high compaction (-0.14%) accommodated during the
403 early stages of localisation at this location. It may also be that this retardation is, in
404 turn, responsible for the relatively late localisation in the overlying strong layer (C) as
405 well as the temporary cessation of movement on the underlying strong layer (E1).
406 Whether these links are causal is unclear, but they suggest that the behaviour at
407 different locations along the localising fault is strongly coupled.

408 (iv) Hanging wall splays – strong layers:

409 These two locations (E2 and G2) straddle what are to become hanging wall splays
410 within the strong layers. Although the faults dip towards the main fault, their sense of
411 shear is in sympathy with the main fault (Fig. 8 and 9c). The two locations show
412 similar strain paths, though again the precise timing of events at each is different.
413 Prior to Mode I failure at these locations (up to 7 - 8cm throw) small linear increases
414 in volumetric strain (up to 0.25%, Fig. 9a) are accompanied by substantial CW
415 rotations (*ca* 1°, Fig. 8 and 9c), rapid decreases in σ_{III} , and slight increases in σ_I (Fig.
416 10a). The significant rotations again record the development of precursory monoclines
417 within the strong layers, a feature which in outcrop studies would generally be
418 referred to as normal drag (e.g. Barnett, et al., 1987; Grasemann et al., 2005). When
419 throws of *ca* 3cm (at G2) and 6cm (at E2) are reached, Mode I fractures develop
420 within the same layers (at G1 and E1 respectively; Fig. 6), along the trend of the
421 incipient main fault, causing stress release and an increase in σ_{III} (Fig. 10a). Even
422 after Mode I failure varying degrees of rotation continue to occur at these locations
423 (Figs. 7 and 9c), a feature, which is attributed to the irregularity of the trace of the
424 newly formed through-going fault. In both cases stress paths are looped or bouncing
425 (Fig. 10a) indicating repeated failure of layers, before rapid increases in volumetric

426 strain (Fig. 9a) and stress release (increase in σ_{III}) correspond to the formation of
427 Mode I fractures (after *ca* 7cm throw at G2, and 8cm throw at E2).

428 In the above discussion we consider only the local stress/strain response
429 within the model. A proxy for the global stress/strain response of the strong layers can
430 be obtained by tracing the strain energy stored in the bonds (i.e. elastic cement) and
431 the bond breakage events. The average strain energy stored in each bond and the total
432 number of broken bonds vs. throw are plotted in Fig. 11a. An initial non-linear
433 increase in strain energy is followed by a slight drop in energy due to failure (and thus
434 removal of bonds) of the lowest layer (G). This drop in energy is accompanied by a
435 large increase in the number of broken bonds (Fig. 11a). After the first failure, both,
436 the strain energy and number of broken bonds increase gradually until the next layer
437 (E) fails. The failure of layer A and C show similar patterns. The drop in strain energy
438 increases with increasing throw and no increase in strain energy is observed after the
439 last strong layer failed (C) and a continuous fault has been established. Following
440 localisation, the strain energy progressively decreases, stabilizing at a value equal to
441 about half the peak value at a throw of 0.5m (not shown).

442 The stress/strain paths and the strain energy/number of broken bonds
443 described above are consistent with conceptual models of fault growth in layered
444 sequences. Fault growth can be summarised as a three-stage process (Fig. 11b):

- 445 1. Monoclinal flexure: Folding is accommodated in the strong layers by elastic
446 bending prior to failure but by flow in the weak layers, which cannot sustain
447 bending moments. Extension and folding leads to horizontal tensile stresses
448 within the strong layers.
- 449 2. Failure of strong layers: Fault segments in the strong layers develop within
450 the precursor monocline. The layers fail in tension and Mode I fractures

451 form. Failure of the strong layers leads to release of tensile stress (increase in
452 σ_{III}) and a rapid increase in volumetric strain. After the first increment of
453 failure, which is pure Mode I, the fractures develop a shear component due to
454 the formation of pull-aparts within the strong layers. Despite the formation of
455 fractures in the strong layers much of the offset is still accommodated by
456 monoclinical folding to provide a zone of fault-related normal drag.

457 3. Formation of through-going fault: After failure of all strong layers a through-
458 going fault develops with localisation of strain in the weak layers, at a throw
459 of *ca* 0.1 m. Segment linkage leads to a staircase-geometry, with steeply
460 dipping fault segments in the strong layers and relatively shallow dipping
461 faults in the weak layers. With the formation of a through-going fault, normal
462 drag becomes progressively less significant with increasing throw so that
463 discontinuous shear displacement accounts for up to 60% and 85% of the
464 total offset at throws of 0.5 and 1m, respectively.

465 It is important to emphasize that only one model is analysed in detail in this study.

466 Different model realisations, with different particle and bond spatial distributions (but
467 identical microproperty statistical distributions) exhibit variable fault geometries due
468 to differences in the locations of stress concentrations causing fracture nucleation.

469 Although the exact locations of fractures and the magnitude and sense of stepping
470 across weak layers will vary between realisations, the overall fault dip and the relative
471 timing and mode of failure (strong layers first as Mode I fractures) is not affected by
472 varying particle and bond spatial distributions.

473

474 **4 Implications for the 3D geometry of faults in multilayer sequences**

475 The ideal conceptual image of a normal fault is that of a continuous surface entirely
476 contained within a volume of rock and bounded by an elliptical tip-line (Watterson,
477 1986; Fig. 3b); more irregular tip-lines are attributed to the interaction with a free
478 surface or other faults (Nicol et al., 1996). For the ideal fault, displacement varies
479 continuously over the fault surface, with contours of displacement concentric about a
480 central maximum. Relative to this simple model, our numerical model is best suited to
481 modelling the displacement accumulation along a vertical chord from the maximum
482 displacement to the upper tip line. For normal faults this chord is characterised only
483 by displacement parallel propagation, with no out-of-plane or lateral propagation (Fig.
484 3b). Although our modelling demonstrates that, at least in its early stages, the
485 localisation of individual faults is, perhaps not surprisingly, more complex than
486 simple models suggest, the general upward progression of deformation away from the
487 maximum displacement does adhere to that of the simple model. This suggestion is
488 developed further by combining interpretations, using both finite (not shown) and
489 incremental maximum shear strain contour diagrams (Fig. 6), of the cross-sections for
490 different throw values of our DEM model, to produce a fence diagram of the fault
491 traces. The fault tip-points on this fence diagram are joined to form continuous fault
492 tip-lines outlining a series of fault segments (Fig. 12) which together represent a fault
493 with a maximum displacement of 10cm at one end and zero displacement on the
494 other. Because the 3D fault plane shown in Fig. 12 is based on 2D modelling, it does
495 not take account of out-of-plane, or lateral, propagation effects, which are likely to
496 increase the complexities associated with fault zone localisation. Nevertheless, the
497 diagram illustrates several interesting features. Firstly, the degree of segmentation
498 decreases with increasing displacement until the segmented array is eventually

499 replaced by a continuous fault. Secondly, despite the segmented nature of the fault, its
500 overall shape approximates to one quadrant of an elliptical fault surface; the retarded
501 localisation within layer C is responsible for the most significant departure from an
502 approximately elliptical form. Thirdly, displacement transfer across contractional
503 steps is possible even when segmented arrays are underlapping, i.e. the structure
504 between beds E and G at a throw of 4 - 8cm. Finally, despite the complex nature of
505 the fault on this scale of observation, the fault segments form a coherent array which,
506 when considered together, resemble a simple single fault. In detail, of course, the
507 segmented fault array shows a tip line that is more advanced in the strong layers
508 (labelled A, C, E and G) than in the weak ones, a feature which suggests that within
509 multilayer sequences tip-lines will, in detail, be fringed. It also shows that linkage of
510 faults in layers C and E via a shallow dipping fault in the intervening weak layer
511 produces a branch point where the segmented array gives way laterally to a
512 continuous fault. Most of all, this geometry emphasizes the fact that the linkage of
513 initially vertically segmented faults does not imply that the faults grew independently,
514 a feature which is consistent with earlier models for segmented fault arrays (Childs et
515 al. 1995, 1996; see also the coherent growth model of Walsh et al. 2003).

516 Our numerical models therefore provide a basis for extending the simple
517 conceptual diagrams of Fig. 2 into 3D. Figure 13 shows that a continuous fault with
518 nearly constant displacements in cross-sectional view can give way laterally to a
519 fringed tip-line in which fault segments within strong layers are more advanced than
520 those within weak layers. For simplicity the block diagram in Fig. 13 considers only
521 segmentation arising from lateral propagation. In reality segmentation will be
522 preserved over an entire fault surface if displacements are not high enough to link
523 between strong layers. An increase in displacement, whether or not it is accompanied

524 by fault propagation, will lead to the progressive replacement of the segmented array
525 by a continuous fault. Even where the fault is segmented we should expect
526 displacements to vary systematically over the fault surface. However, when account is
527 taken of both the discontinuous displacements on the fault and the continuous
528 displacements accommodated by fault-related ductile deformations adjacent to the
529 fault, displacement variations are reduced. In proportional terms, ductile deformation
530 is likely to be more significant early in the localisation process, when fault segments
531 remain unlinked. Continuity of displacement and related strains reflects the
532 underlying fact that segments within an initially segmented array form a geometrically
533 and kinematically coherent system, in which neither the displacements nor the
534 locations of segments are incidental (coherent growth model, Walsh et al., 2003; see
535 also Childs et al. 1995).

536

537 **5 Discussion**

538 The Discrete Element Method (DEM), as implemented in *PFC-2D*, has been used to
539 model the growth of a normal fault in a brittle/ductile multilayer. The principal
540 advantage of the DEM compared to continuum methods (Finite Element, Finite
541 Difference and Boundary Element Methods) is that discrete fractures and faults with a
542 large finite displacement can be more effectively modelled; advances in combined
543 approaches (DEM-FEM) may, however, provide better means for future fault and
544 fracture modelling. The main limitations in the modelling approach in this study are
545 that the model materials are strain-rate independent and that fluids and their effects
546 (e.g. over-pressuring, precipitation of minerals) are neglected. Despite these
547 limitations, the modelling is capable of reproducing many of the characteristic
548 features of natural faults, providing a mechanical rationale for their geometry and

549 growth. In particular, it provides a basis for investigating whether normal faults in
550 layered sequences localise first in the strong layers or the weak layers (Ferrill and
551 Morris, 2003), a question that cannot be addressed using conventional mechanical
552 analyses such as Mohr diagrams (Mandl, 2000).

553 The DEM models presented in this article incorporate properly calibrated
554 model materials that reproduce the behaviour of natural rocks. The brittle/ductile
555 multilayer sequence comprises strong layers, which are brittle at low to intermediate
556 confining pressures and have elastic properties and strengths similar to those of strong
557 sedimentary rocks, interbedded with weak layers, which are cohesionless, frictional-
558 plastic, and cannot sustain bending moments. Faulting in such a layered sequence
559 leads to an increase in layer parallel tensile stress (decrease in σ_{III}) and an increase in
560 volumetric strain in the strong layers until the material fails in tension (Mode I).
561 Diffuse zones of pure shear dominated deformation (squeeze flow) in the weak layers
562 accommodate small amplitude precursor folding of the strong layers prior to failure.
563 Deformation in these zones has a small rotational component which is antithetic with
564 respect to the main fault, and is in that respect similar to the antithetic ‘damage zones’
565 at the tip of faults in homogeneous, non-layered rocks described by Kim et al. (2003).
566 Although both types of antithetic faults form within a zone of distributed shear, the
567 geometries of antithetic faults in our DEM models are strongly affected by layering,
568 in that they link the hinges of a fault related monocline. In our model Mode I fractures
569 within the strong layers form an initial vertically segmented fault array which is later
570 linked via shallow dipping faults in the weak layers. The model results provide a
571 mechanical basis for fault refraction arising from different modes of faulting within
572 different layers, with tensile failure in the strong layers and shear failure in the weak
573 layers. At overburden pressures greater than that applied here ($> ca$ 100MPa) the

574 strong layers in this model fail in shear rather than in tension, but even in these
575 circumstances faults tend to initiate first within the strong layers and the fault zone is
576 an initially vertically segmented array. As in the low effective stress model the fault
577 dips within the strong layers are controlled by the failure mode, whereas the fault dips
578 within the weak layers are mainly controlled by segment linkage.

579 The model suggests also that abandoned fault tips or splays are not essential
580 features of an initially vertically segmented array. Fault segments which underlap and
581 do not generate abandoned tips and splays when they link, can form coherent arrays
582 and show complementary displacement transfer, provided the intervening volume can
583 accommodate ductile strains. The model highlights the fact that the initially vertically
584 segmented fault array is geometrically and kinematically coherent (Walsh and
585 Watterson, 1991; Walsh et al., 2003) and that the fault segments do not grow
586 independently in individual layers (Benedicto et al., 2003) but could link laterally into
587 a continuous fault (fig. 9 in Childs et al., 1996).

588 The model also demonstrates that initial Mode I fracturing is not necessarily
589 an indicator of high pore pressure (as suggested for example by McGrath and
590 Davison, 1995). Fluid pressure only increases the depth of possible tensile failure
591 since it decreases the effective stress. Fault refraction at low effective stress is not
592 'due to high pore pressure' but due to different types of failure (extension vs. shear) in
593 the different lithologies (Peacock and Sanderson, 1992). The suggestion that fault
594 segmentation is a product of fault propagation (e.g. Jackson, 1987; Mandl, 1987; Cox
595 and Scholz, 1988; Peacock and Zhang, 1993, Childs et al., 1996, Walsh et al., 2003,
596 Marchal et al., 2003) is supported by DEM modelling, though the importance of
597 mechanical layering in controlling segmentation cannot be overstated.

598

599 **6 Conclusions**

600 The Discrete Element Method (DEM), as implemented in *PFC-2D*, has been used for
601 modelling the growth of a normal fault within a brittle/ductile multilayer sequence.

602 Our research suggests that the DEM is capable of modelling the failure and
603 localisation processes of faulting, aspects that cannot be modelled adequately using
604 conventional continuum based methods. Our modelling provides new insights into
605 both the mechanics and kinematics of faulting at low effective stresses and suggests
606 the following principal conclusions:

- 607 • Large dip variations, and related fault refraction, are due to different types of
608 failure (extension vs. shear) of layers.
- 609 • Normal faults in brittle/ductile sequences localise first in strong layers as
610 steeply dipping Mode I fractures and are later linked via shallow dipping
611 faults in weak layers.
- 612 • Faults contained in multilayer sequences have fringed tip lines, where the
613 fault is laterally more advanced in the strong layers than in the weak layers.
614 The extent of fringing is a function of strength contrast between the layers
615 and fault displacement.
- 616 • Models for the 3D segmentation of faults in sedimentary sequences must
617 include the effects of rock properties and mechanical layering.

618

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634

635 **Appendix A**

636 *Mohr Circles for \mathbf{D}*

637 An extremely useful graphical representation of the position gradient tensor is the
638 Mohr circle for \mathbf{D} (e.g. Means, 1983 and 1990).

639 Any two-dimensional, homogeneous deformation can be written as

640

$$641 \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} D_{11} & D_{12} \\ D_{21} & D_{22} \end{pmatrix} \begin{pmatrix} X_1 \\ X_2 \end{pmatrix} \quad (\text{A-1a})$$

642

643 or more compactly as

644

$$645 \mathbf{x} = \mathbf{DX}, \quad (\text{A-1b})$$

646

647 where \mathbf{X} and \mathbf{x} are position vectors for a particle in the undeformed and
648 deformed state, respectively, and D_{11} , D_{12} , D_{21} and D_{22} are the components of the
649 position gradient tensor \mathbf{D} , which contains information about the stretch and rotation
650 and is referred to as the deformation tensor in this Appendix.

651 The components of \mathbf{D} can be obtained by deforming a unit square into a
652 parallelogram (Fig. A-1a). Components D_{11} and D_{21} are determined using the x_1 and
653 x_2 coordinates of the corner point that was located at (1,0) whereas components D_{12}
654 and D_{22} are obtained using the x_1 and x_2 coordinates of the corner point that was
655 located at (0,1) in the undeformed state.

656 A Mohr circle (of the first kind; De Paor and Means, 1984) representing \mathbf{D} is
657 drawn using equally calibrated axes for the normal (D_{11} , D_{22}) and shear components
658 (D_{12} , D_{21}). Two points are plotted at (D_{11} , $-D_{21}$) and (D_{22} , D_{12}), connected by a line
659 and a circle is drawn about this line (Fig. A-1b). The polar co-ordinates of any point
660 on the \mathbf{D} circle gives the stretch and rotation of a material line.

661 The principal stretches, s_I and s_{III} ($s_I > s_{III}$) can be graphically obtained by
662 intercepting the circle with a line drawn from the origin through the centre of the
663 circle (Fig. A-1b). The diameter of the Mohr circle is therefore related to the intensity
664 of stretching, since the ellipticity of the strain ellipse is s_I/s_{III} . The volumetric strain
665 (strictly speaking area change), which cannot be directly read off the Mohr diagram, is
666 the product of the principal stretches minus one.

667 Symmetric deformation tensors ($D_{12} = D_{21}$) represent irrotational
668 deformation and Mohr circles have their centre on the horizontal axis (Fig. A-2b and
669 d). Mohr circles of this kind are often referred to as Mohr circles for stretch.
670 Asymmetrical deformation tensors ($D_{12} \neq D_{21}$) represent rotational deformation (Figs.
671 A-1, A-2a and c). The rotational component of any strain is given by

672

673
$$\tan \omega = \frac{D_{21} - D_{12}}{D_{11} + D_{22}} \quad (\text{A-2})$$

674

675 and can be obtained graphically by measuring the angle between a line drawn
676 from the origin to the centre of the circle and the horizontal axis, where by definition
677 clockwise rotation is negative (Fig. A-1b). Off-axis circles centred above the
678 horizontal axis represent deformation with a clockwise (by convention negative)
679 rotational component (Fig. A-2a and c).

680 Rigid body rotation leads to circles with zero radius and centres on a unit
681 circle in the Mohr diagram (Fig. A-2e). In this study it has proven useful to plot a unit
682 circle with its centre in the origin and lines with slopes in 1° intervals (Fig. 8). These
683 guidelines assist in estimating the amount of rigid body rotation prior to stretching.

684 The maximum angular shear strain is given by

685

686
$$\tan \psi_{\max} = \frac{s_I^2 - s_{III}^2}{2s_I s_{III}} \quad (\text{A-3})$$

687

688 and can be obtained graphically by drawing a chord through the centre of the
689 circle perpendicular to the line that passes through the principal stretches (Fig. A-1b).
690 The intersection of the chord with the circles gives the points that represent material
691 lines that were perpendicular to each in other in the undeformed state (as usual double
692 angles are measured in Mohr circles). This pair of lines experienced the maximum
693 shear strain, since they are symmetrically arranged with angles of $\pm 45^\circ$ to the principal
694 stretches in the undeformed state (Fig. A-1b).

695

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800

801 **Figure captions**

802

803 **Figure 1:** A small-scale normal fault (displacement = 30cm; downthrows to the right)
804 exposed in a cliff-section east of Kimmeridge Bay, Dorset, UK, which illustrates the
805 importance of lithological control on fault dip and fault refraction. This normal fault
806 cuts a shale-dominated sequence (Kimmeridge Clay Formation, Upper Jurassic) that
807 contains calcareous shale layers. Within these calcareous shales fault segments are
808 nearly vertical and are linked via shallow dipping faults within the weaker shale
809 layers. Fault displacement on this ‘staircase’ geometry leads to the development of
810 pull-aparts.

811

812 **Figure 2:** (a) Schematic geometry of normal faults cutting limestone layers of the
813 Cretaceous Buda Limestone exposed along Interstate Highway 10 (I-10), in west
814 Texas and three possible models for their growth (b, c and d; after Ferril and Morris,
815 2003; table 1 and fig. 5). In (b) the faults localise first in the strong layers and the
816 steep segments are later linked via shallow faults. In (c) the faults localise first in the
817 weak layers and the shallow segments become linked via steep faults. In (d) the fault
818 trace is not initially segmented but the trajectory of the upward propagating fault tip
819 changes as it crosses a lithological interface, i.e. a bedding plane.

820

821 **Figure 3:** Model boundary conditions. (a) *PFC-2D* model consisting of >23,400
822 cylindrical particles. The strong and weak layers consist of bonded and non-bonded
823 particles, respectively (bonds are shown in enlarged figure). Confining pressure is
824 approximately 23MPa and the hanging wall moves with constant velocity parallel to a
825 predefined fault at the base of the model. (b) Schematic block diagram showing the

826 propagation directions of an ideal elliptical normal fault. The tip line bounds an
827 elliptical area of failed rock (white). Since the fault plane propagates radially (arrows
828 show tip line propagation direction) only two sections (shaded) have no out-of-plane
829 fault propagation. The 2D numerical model is located within the plane of no lateral
830 fault propagation. This fault is shown schematically as a single fault surface, but in all
831 probability will comprise an array of segments.

832

833 **Figure 4:** (a to d) Plots illustrating the results of rheological testing of the strong (a
834 and c) and weak (b and d) materials comprising the multilayer models at various
835 confining pressures (labelled curves). Vertical dashed lines in are drawn at 0.3, 0.4
836 and 0.5% axial strain. (e and f) Contour plots showing the distribution of maximum
837 finite shear strain (contour interval is 0.005) within models comprising the strong (e)
838 and weak (f) materials at axial strains of 0.3, 0.4 and 0.5% and a confining pressure of
839 25MPa.

840

841 **Figure 5:** Principal stress diagram with best-fit failure envelopes (bold lines) for the
842 strong and weak material. The data for the strong material were obtained from direct
843 tension tests on dog-bone shaped samples with a central width of 1m at various
844 confining pressures and each data point represents the state of stress at failure ($N =$
845 196). The data for the weak material were obtained from confined (25MPa) biaxial
846 compression tests and each data point represents the peak stress during loading ($N =$
847 30). The best-fit macroproperties are given, where σ_{uc} = unconfined compressive
848 strength (MPa), T = tensile strength (MPa), C_0 = cohesion (MPa) and μ = friction
849 coefficient. For the strong material the different curves represent the 0.01, 0.5, 0.25,
850 0.50, 0.75, 0.95 and 0.99 percentile of the probability distribution. For the weak

851 material the average friction coefficient and the average ± 1 and ± 2 standard
852 deviations are shown.

853

854 **Figure 6:** Incremental maximum shear strain contour plots (contour interval is 0.005)
855 of a *PFC-2D* model of normal fault growth in a brittle/ductile sequence ($t = \text{throw}$).

856 The different layers within the model are labelled A to H. See text for further
857 explanation.

858

859 **Figure 7:** Strain profiles in 2cm throw increments (labelled in **b**) along the centre of
860 layer E. The maximum finite shear strain (**a**) and the rotational component of

861 deformation (**b**) were obtained for 1m wide circular homogenisation regions with
862 10cm spacing. The two vertical dashed lines are the locations of Mode I fractures

863 (labelled E1 and E2; see Figs. 6 and 8). The plateaux of the curves in (**b**) correspond
864 to the limb of the monocline, the left hand hinge of which fails at between 5cm and
865 6cm throw.

866

867 **Figure 8:** Strain paths at selected locations (circled regions labelled A - H) in the
868 multilayer model. The central diagram is of the multilayer model at a finite throw of
869 10cm which is contoured for maximum finite shear strain (contour interval is 0.01).

870 Individual beds within the multilayer are labelled A to H. Mohr circles for finite strain
871 at 1cm throw increments are illustrated; arrows connect centres of successive Mohr

872 circles. The dashed vertical arc in each Mohr diagram is part of a unit circle with its
873 centre located at the origin. The centres of Mohr circles for rigid body rotation plot on

874 this arc. The dash-dot lines are lines intersecting the origin with slopes in 1° intervals
875 (labelled in B). These guidelines can give quick insights into rotations (e.g. 1° CW

876 rigid body rotation prior to formation of pull-apart as in diagram G2). See text and
877 Appendix A for further explanation.

878

879 **Figure 9:** Graphs of volumetric strain (**a** and **b**) and the rotational component of
880 deformation (**c** and **d**) vs. throw for the locations labelled in Fig. 8.

881

882 **Figure 10:** Principal stress paths for the locations labelled in Fig. 8 with
883 experimentally derived failure envelopes (Fig. 5). Each arrow corresponds to the
884 change of stress in a 1cm throw increment and dots represent the state of stress prior
885 to faulting.

886

887 **Figure 11:** Three-stage development of fault growth in a multilayer sequence as
888 illustrated by (**a**) plot of number of broken bonds and average strain energy per bond
889 vs. throw recorded in the model shown in Fig. 6 and (**b**) schematic representation of
890 stages in development of the same model. The data in (**a**) were obtained from the
891 model by tracking each bond breakage event and the strain energy stored in the bonds.
892 The onset of failure of each strong layer is labelled and marked with vertical dashed
893 lines. In (**b**) monoclinical flexuring is exaggerated and only localised deformation is
894 shown. The precursor zone of faulting (bounded by the two dashed lines) is idealised
895 as a planar feature, whereas the modelled zone broadens upwards due to the
896 predefined nature of the fault at the base of the model and free surface effects.

897

898 **Figure 12:** 3D fault plane constructed from interpreted fault traces from the *PFC-2D*
899 model shown in Fig. 6 assuming the temporal fault zone evolution is equivalent to
900 spatial variation in fault zone structure with increasing displacement. Labelled layers

901 (A, C, E and G) are strong layers. To construct this diagram, the lateral displacement
902 gradient was taken as 1:150, i.e. 1.5m distance along strike between successive
903 sections in Fig. 6. The fault is typically more advanced in the strong layers; the
904 advancement within layer C is approximated, since no section is available at a throw
905 of 8.5cm.

906

907 **Figure 13:** Conceptual growth model for normal faults cutting limestone layers of the
908 Buda Limestone (see Fig. 2). The block diagram is located at a lateral fault tip (Fig.
909 3b). For simplicity the fault is shown with no vertical displacement gradient. The
910 block diagram was constructed using cross sections shown in Fig. 2a and b.

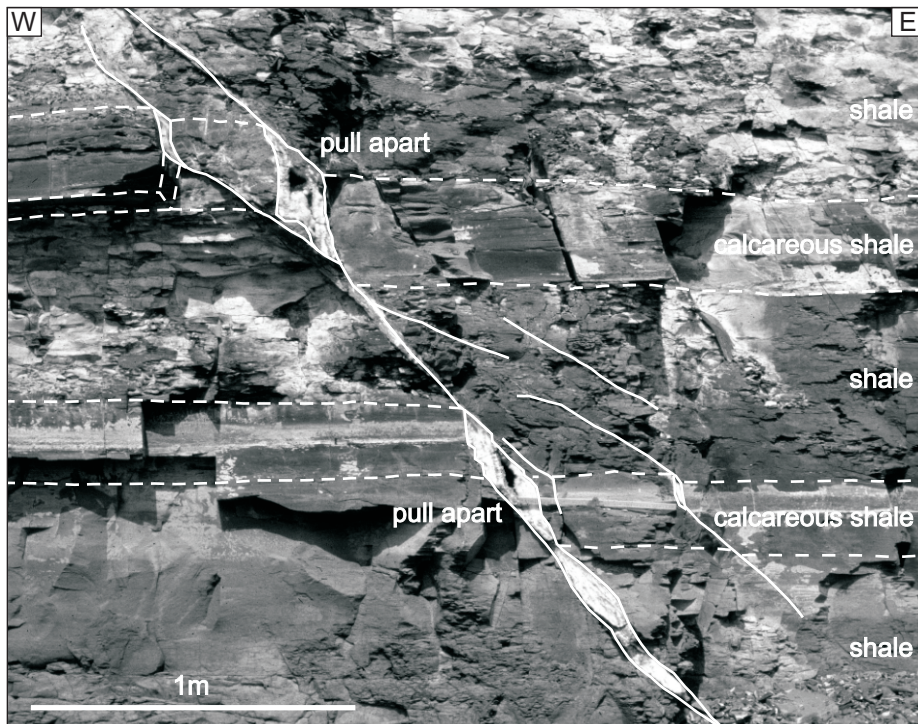
911

912 **Figure A-1:** Plotting and reading Mohr circles for **D**. (a) The components of the
913 deformation tensor (D_{11} etc.) are derived from the corners of the deformed unit square
914 as shown. The deformation tensor for this parallelogram is also given. (b) Mohr circle
915 representation of the **D** tensor. The constructions for finding the principal stretches, s_I
916 and s_{III} , the rotational component of deformation, ω , and the maximum angular shear
917 strain, ψ_{max} , are illustrated. See Appendix A for further explanation.

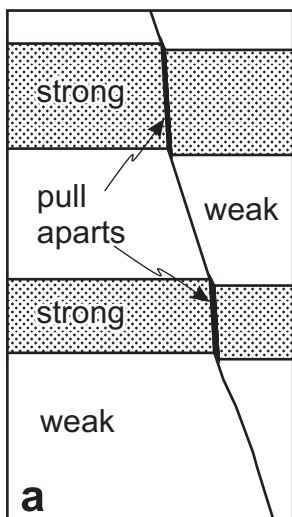
918

919 **Figure A-2:** Illustrations of Mohr circles for deformation, **D**, for a range of strain
920 paths. For each labelled example the Mohr circles and the corresponding deformed
921 unit square in Cartesian coordinates (dotted lines) are shown (the finite state of strain
922 is shown as solid lines and intermediate stages are shown as dashed lines). Strain
923 paths in (a), (b) and (c) are constant volume deformation. The strain path shown in (d)
924 is irrotational simple extension (dilation), (e) is rigid body rotation without stretching.
925 and (f) is rigid body rotation (e.g. normal drag in the context of faulting) followed by

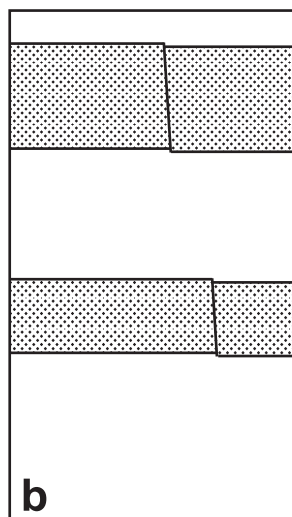
926 simple extension (e.g. the formation of a Mode I fracture). In **(d)** and **(f)** only one set
927 of parallel lines exists that shows neither finite nor incremental stretch.



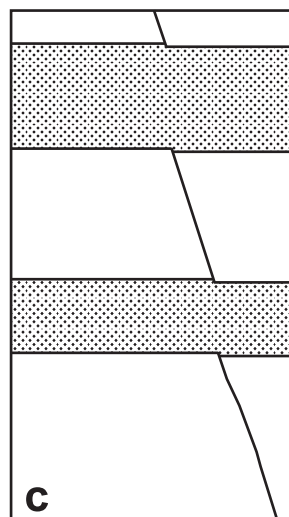
final fault geometry



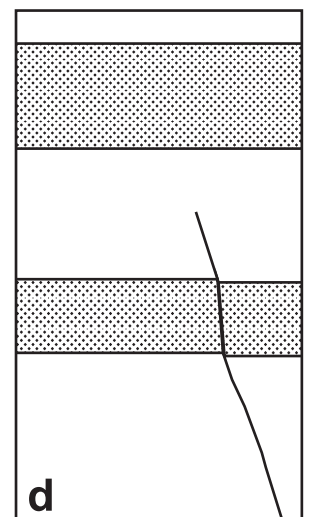
strong layers first



weak layers first

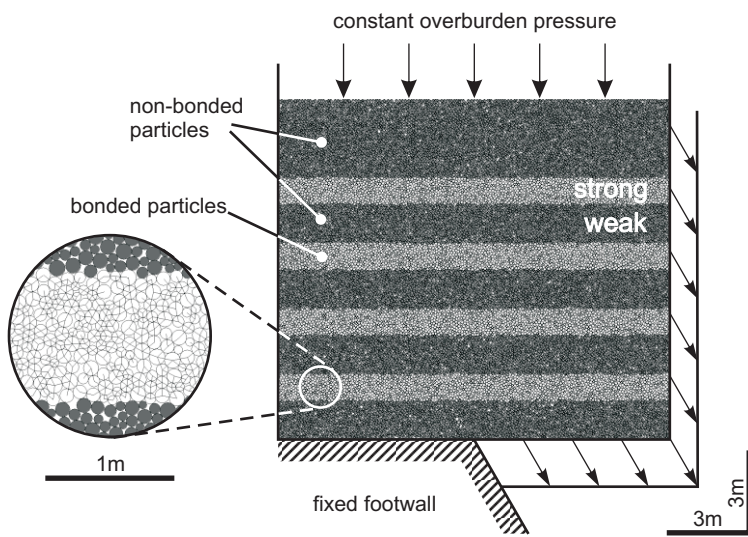


forward propagation

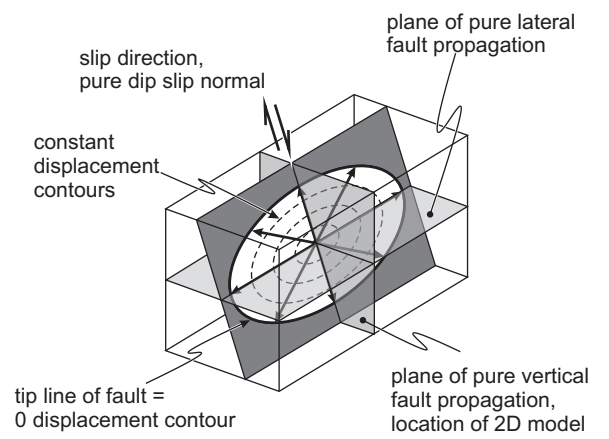


5m

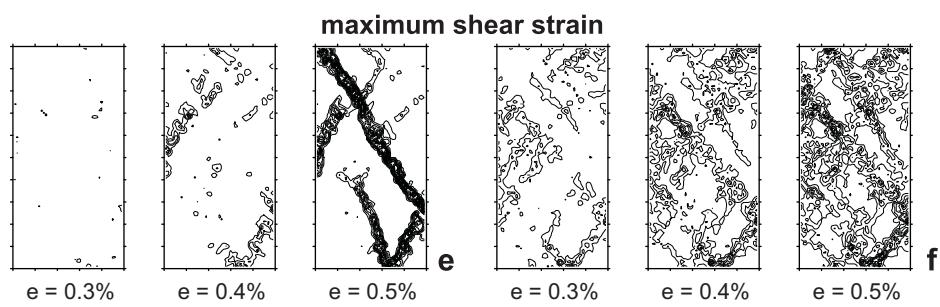
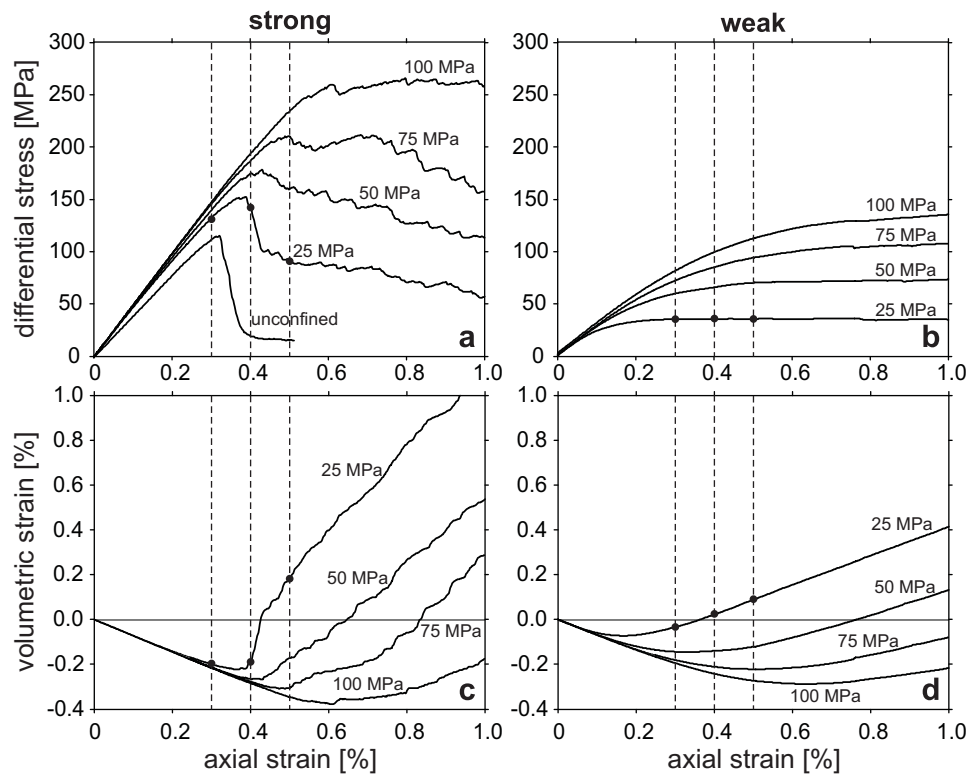


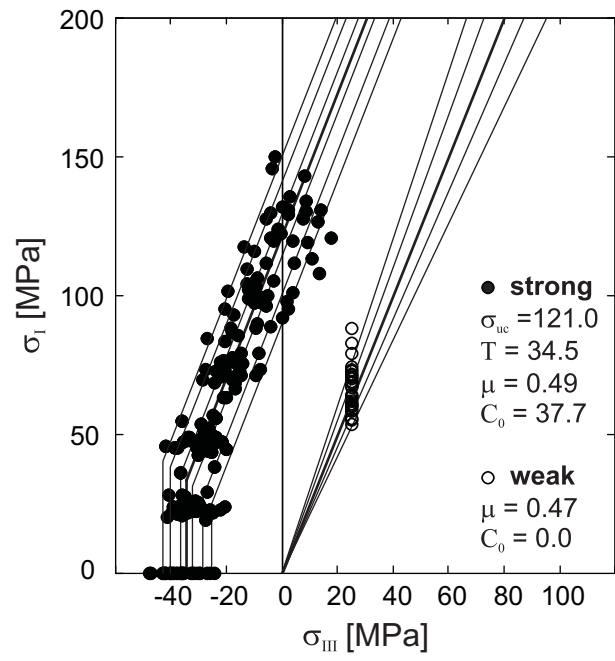


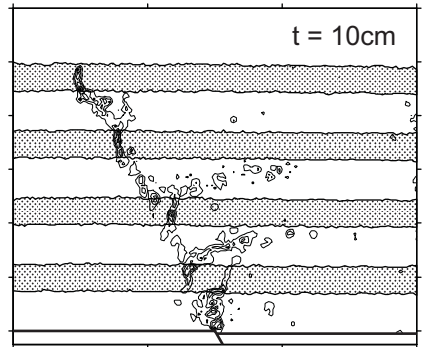
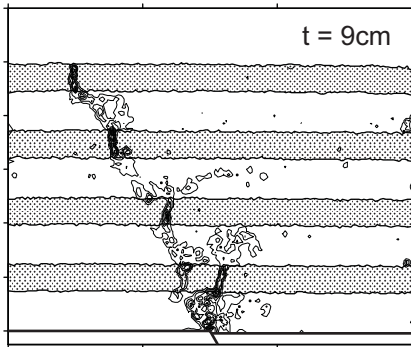
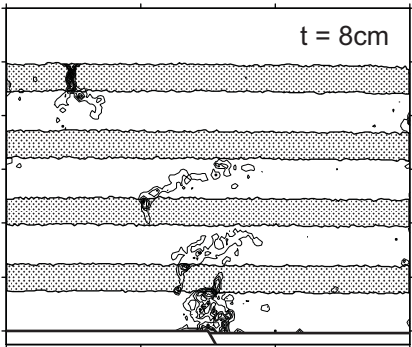
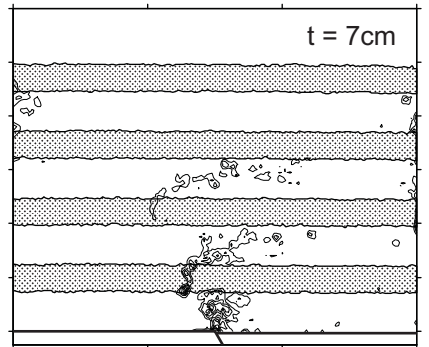
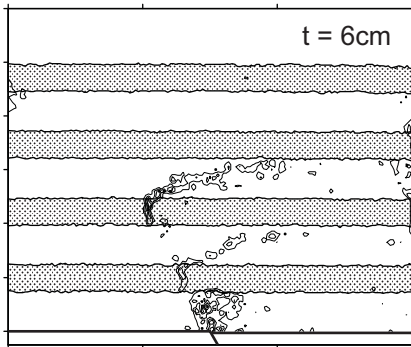
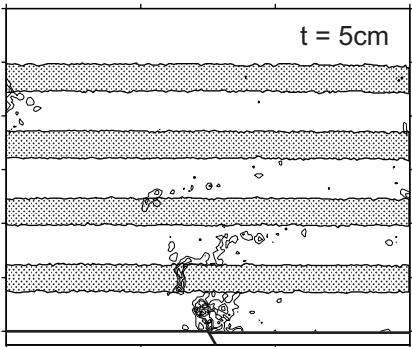
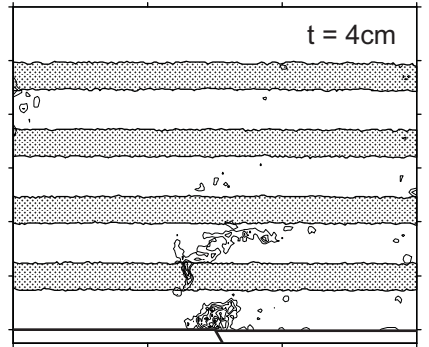
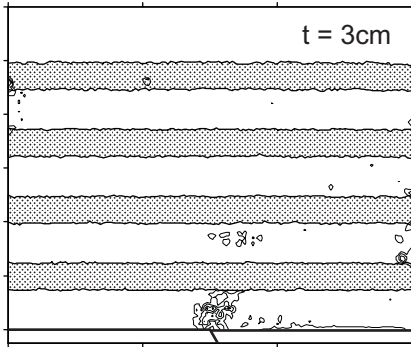
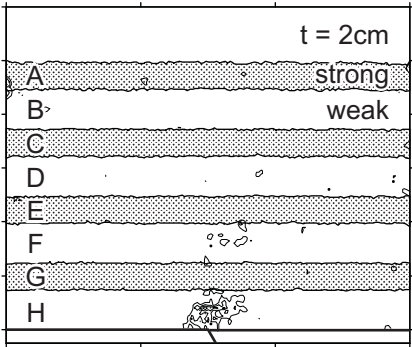
(a)



(b)

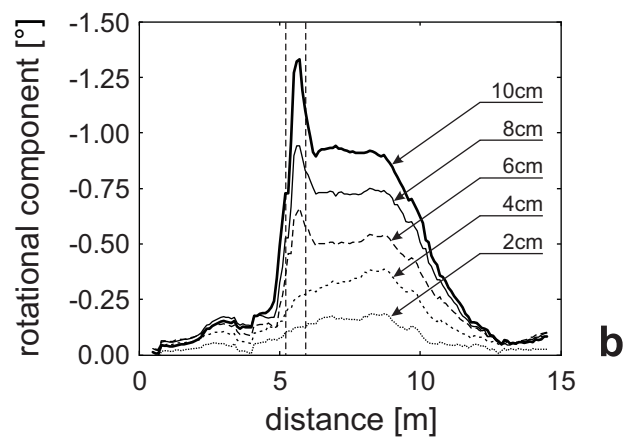
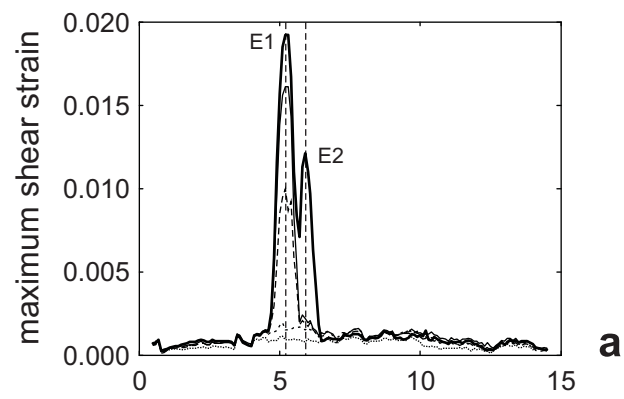


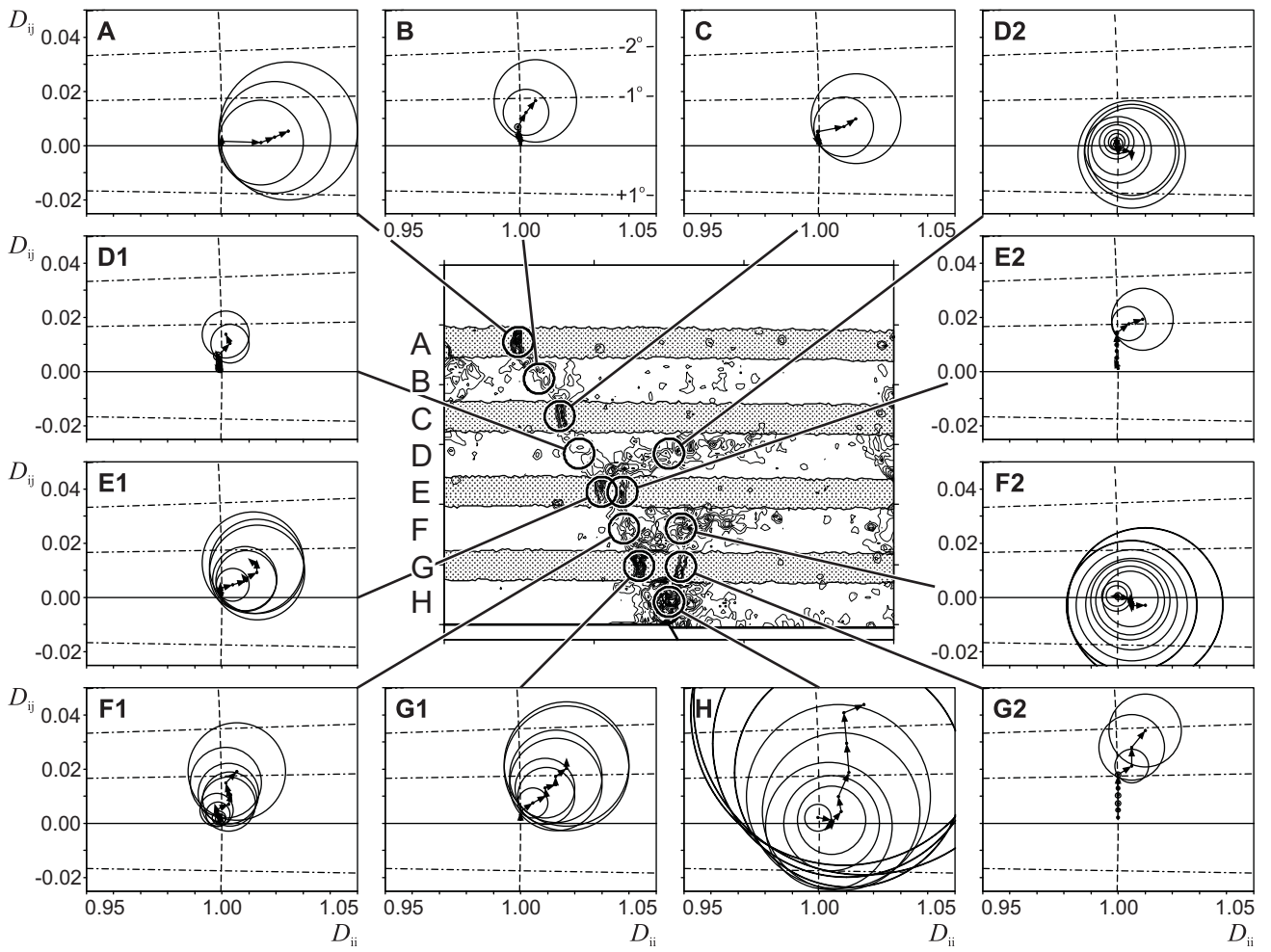


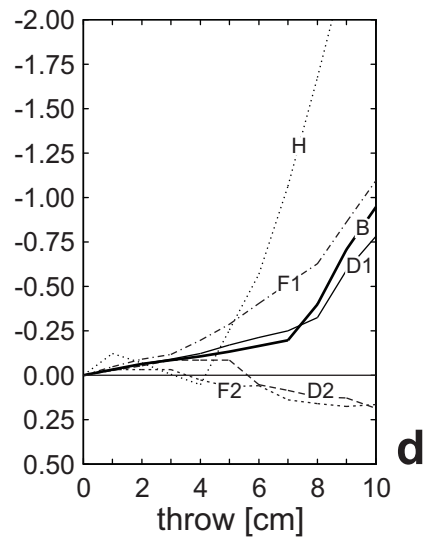
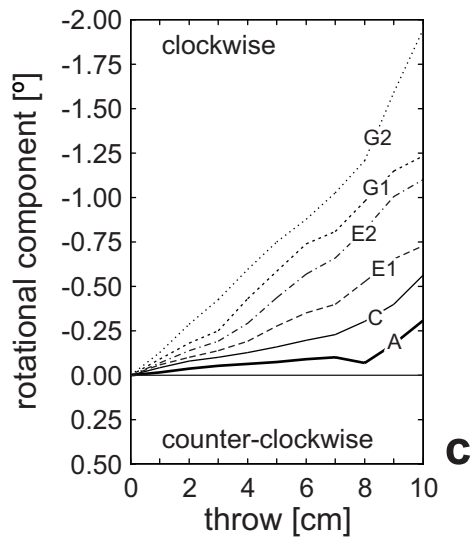
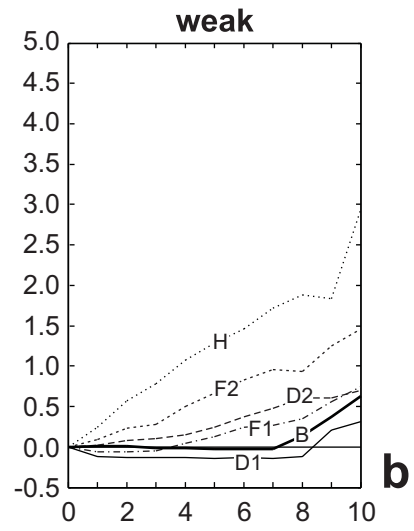
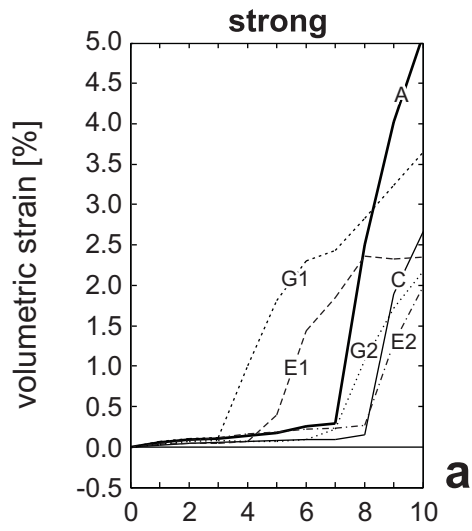


10m

A horizontal scale bar representing 10 meters.

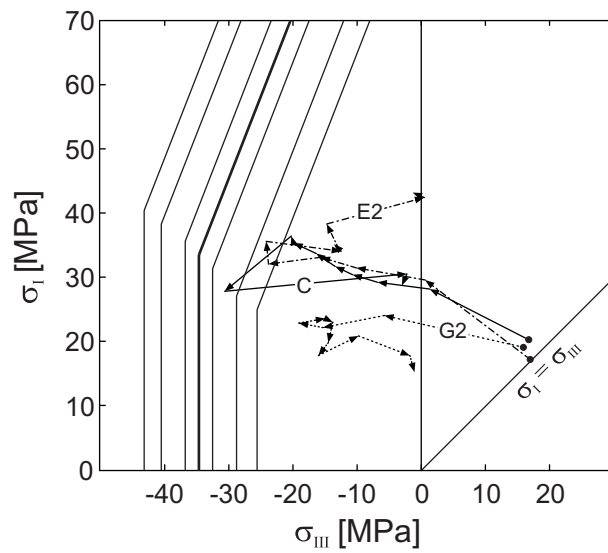
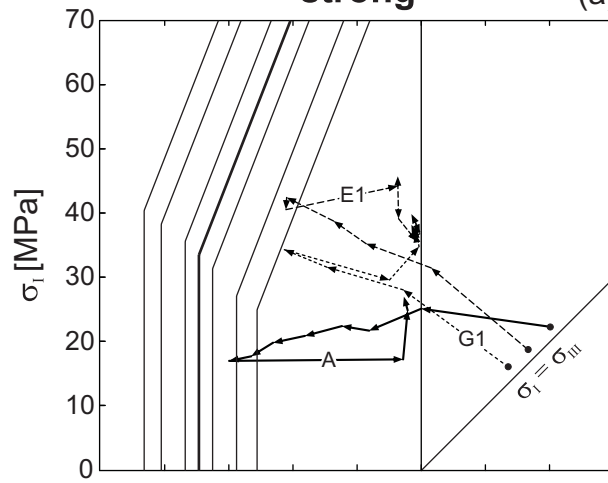






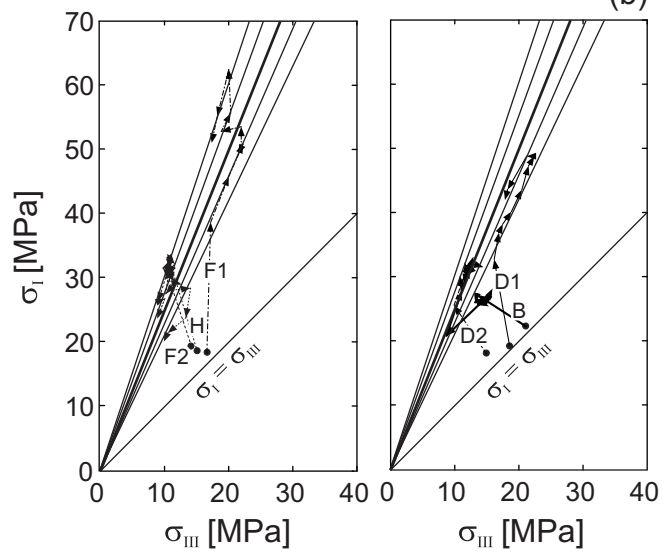
strong

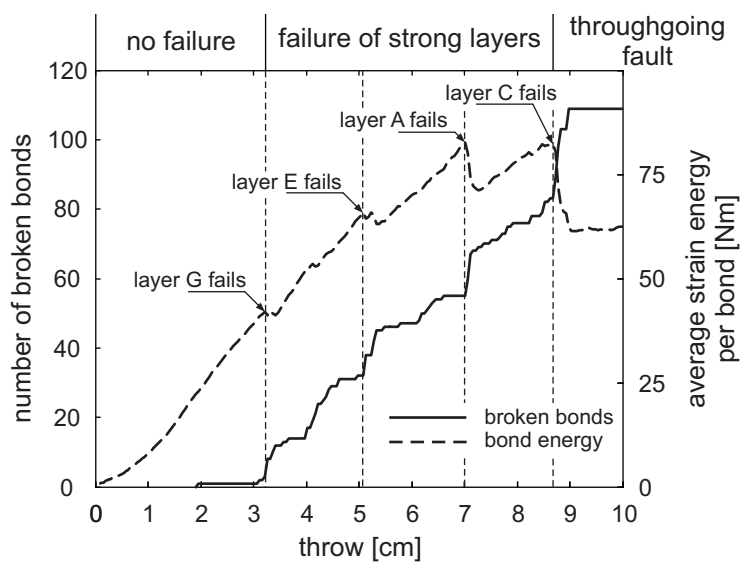
(a)



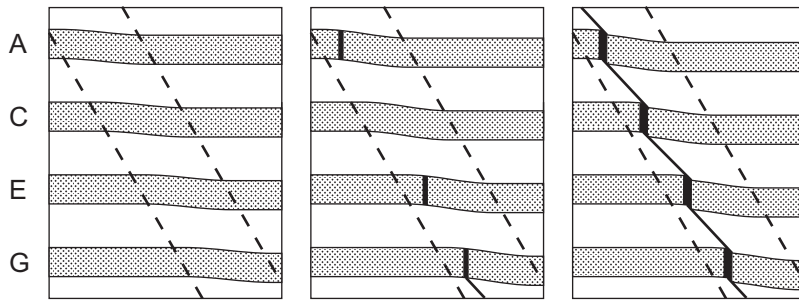
weak

(b)

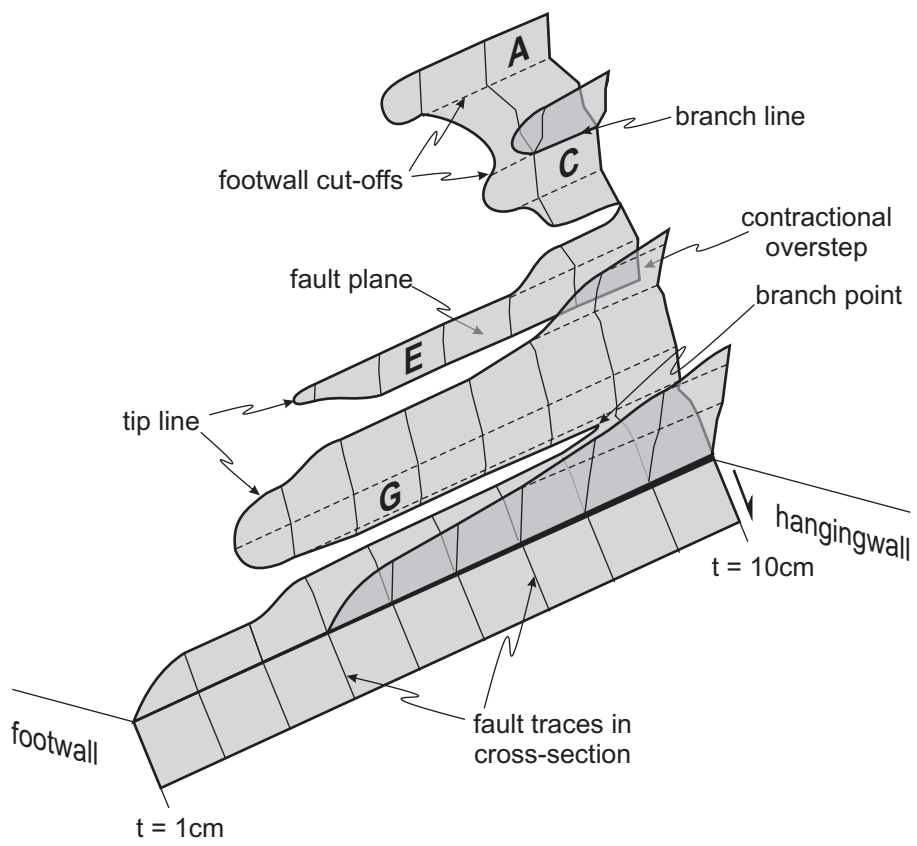


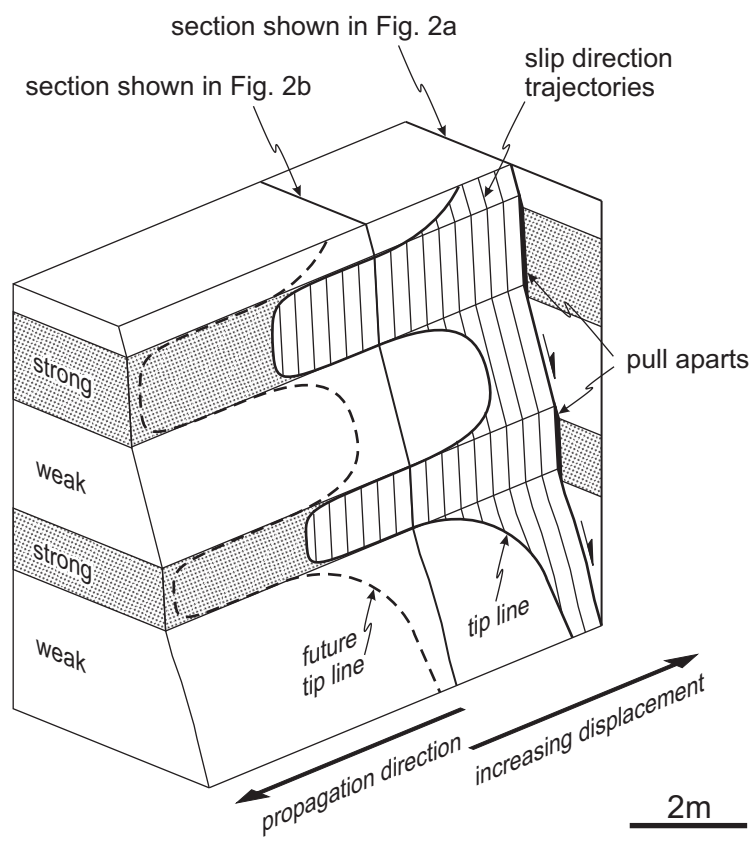


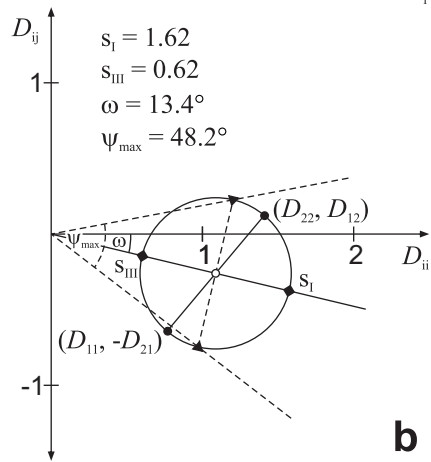
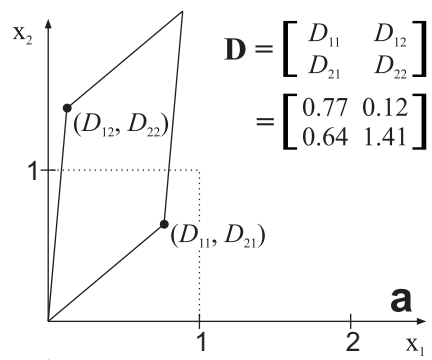
a

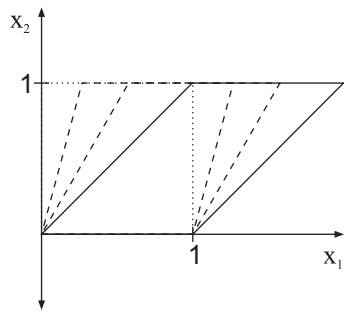


b

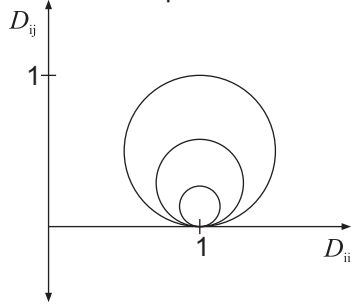




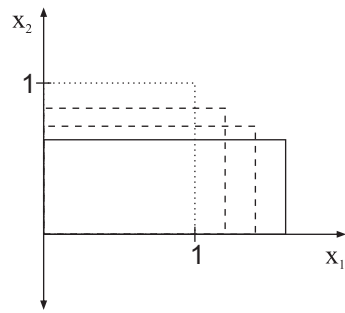




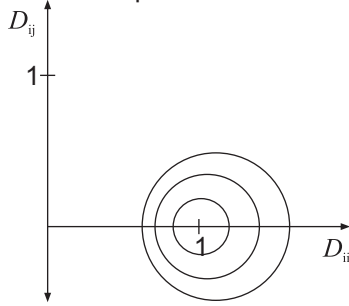
simple shear



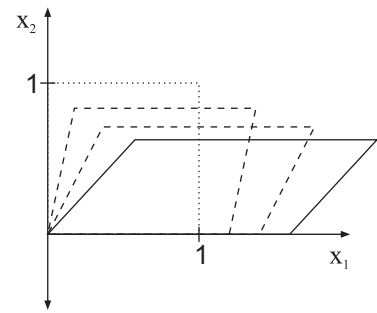
a



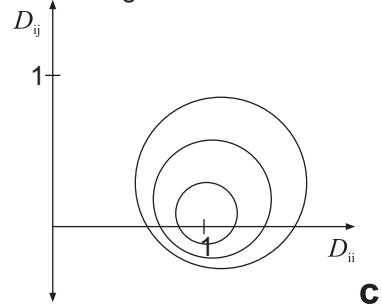
pure shear



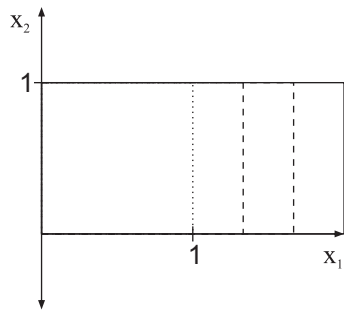
b



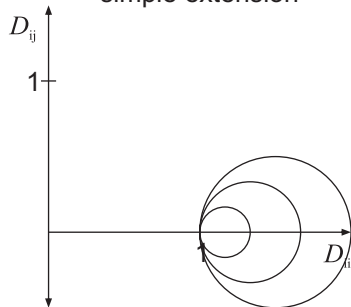
general shear



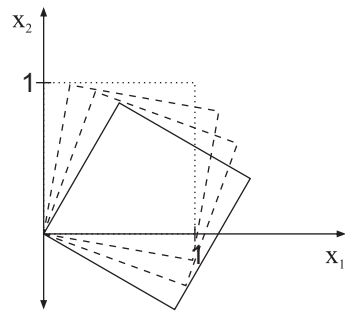
c



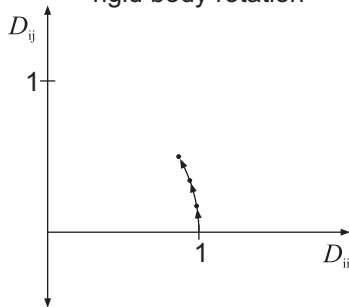
simple extension



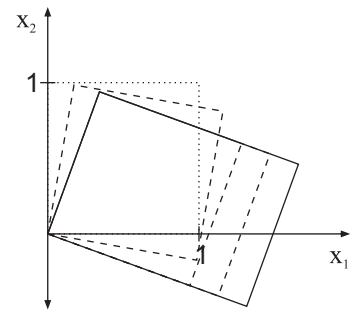
d



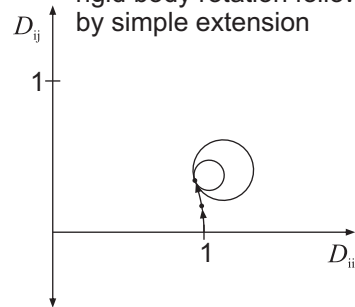
rigid body rotation



e



rigid body rotation followed by simple extension



f