- 1 De-risking the energy transition by quantifying the uncertainties in fault stability
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14 Abstract

15 The operations needed to decarbonise our energy systems increasingly involve faulted rocks in the 16 subsurface. To manage the technical challenges presented by these rocks and the justifiable public concern 17 over induced seismicity, we need to assess the risks. Widely used measures for fault stability, including slip 18 and dilation tendency and fracture susceptibility, can be combined with Response Surface Methodology from 19 engineering and Monte Carlo simulations to produce statistically viable ensembles for the analysis of 20 probability. In this paper, we describe the implementation of this approach using custom-built open source 21 Python code (pfs – probability of fault slip). The technique is then illustrated using two synthetic datasets and 22 two case studies drawn from active or potential sites for geothermal energy in the UK, and discussed in the 23 light of induced seismicity focal mechanisms. The analysis of probability highlights key gaps in our knowledge 24 of the stress field, fluid pressures and rock properties. Scope exists to develop, integrate and exploit citizen 25 science projects to generate more and better data, and simultaneously include the public in the necessary 26 discussions about hazard and risk.

27

28 Introduction

29 Rationale & Objectives

30 Faults in the crust slip in response to changes in stress or pore fluid pressure, and the source of these changes 31 can be either natural or anthropogenic. Estimating the likelihood of slip on a particular fault for a given 32 change in loading is critical for the industrial operations of the energy transition, especially geothermal 33 energy and carbon sequestration and storage (CCS). The target formations of these operations are nearly 34 always faulted and fractured to some degree, and experience from waste-water injection in the USA shows 35 how even small changes in pore fluid pressure can trigger frequent seismic slip on these faults, with 36 significant and widespread impact on society (e.g., Elsworth et al., 2016; Hincks et al., 2018; Hennings et al., 37 2019).

38 Stephenson et al. (2019) have shown how quantitative analysis of the subsurface is one of the key 39 contributions that geoscientists can make to decarbonising energy production to meet national and 40 international targets (e.g., CCC, 2019; IPCC, 2018). This includes the systematic geomechanical 41 characterisation of rock formations, better understanding of fluid flow in fractured rocks, and the need for 42 pilot projects to explore the scaling of behaviours from the laboratory to the field. Perhaps the most 43 important aspect is to understand the public attitudes to subsurface decarbonisation technology 44 (Stephenson et al., 2019; Roberts et al., 2021). Several recent studies have addressed the uncertainties in 45 subsurface structural analysis of faulted rocks (Bond, 2015; Alcalde et al., 2017; Miocic et al., 2019). In this paper, we extend this work to specifically include fault stability, and argue that in order to simultaneously 46 47 address public concerns and assess the viability of different schemes, we need a more rigorous approach to 48 risking subsurface decarbonisation activities, especially where these involve changes in load on faulted rocks.

Useful measures of fault stability include slip and dilation tendency (*T*_s and *T*_d respectively) and fracture susceptibility (*S*_f, the change in fluid pressure to push effective stress to failure). These measures are defined as functions of the *in situ* stress, the orientation of the fault plane and, in the case of *S*_f, rock properties. It is widely recognised that the inputs for the prediction of stability are always uncertain, and to varying degrees: e.g., the vertical stress component of the *in situ* stress tensor can often be quite well constrained (to within

5%) from density log data, whereas the maximum horizontal stress is generally much harder to quantify. To

improve and focus our predictions of fault stability in the subsurface, we need to accept and incorporate

these uncertainties into our calculations. In this paper, we describe and explore a statistical approach to fault

57 stability calculations, and then apply these methods to examples in geothermal energy, in both low- and

58 high-enthalpy settings.

59 The specific aims of this paper are to:

60 1. describe and explain the Response Surface Methodology, and show how it can be applied to the61 probabilistic estimation of fault stability using a range of different measures;

explore how the main variables – in situ stress, fault orientation and rock properties – relate to the different
 measures of fault stability (*T_s*, *T_d* and *S_f*) using synthetic (i.e., artificial) data;

3. use case studies of active and proposed geothermal projects with publicly available data to illustrate the
 method, and then highlight the relationships between our known but uncertain input data and the predicted
 risk of fault slip.

67 Importance & Previous work

68 Small changes in stress or fluid pressure (e.g., a few MPa) from human activities can have significant 69 consequences for fault stability. For example, waste-water injection from hydraulic fracturing ("fracking") 70 operations has led to dramatic increases in seismicity in Oklahoma since 2009 (Hincks et al., 2018) and in 71 Texas since 2008 (Hennings et al., 2019; Hicks et al., 2021). The precise mechanical cause(s) of this seismicity 72 is the subject of some debate, and could be due to either 'direct' pore fluid pressure transfer to basement-73 hosted faults leading to a reduction in effective stress, or 'indirect' poroelastic effects at a distance (Elsworth 74 et al., 2016; Goebel et al., 2019). The concept of critically stressed faults in the crust (Townend & Zoback, 75 2000), where relatively high permeability serves to maintain near-hydrostatic pore pressures, is consistent 76 with the idea that only minor perturbations in loading can have dramatic consequences, even in areas of 77 apparently low seismicity and, implicitly, low background tectonic loading.

78 In densely populated areas such as the UK, public support for, and confidence in, subsurface operations are 79 key. Hydraulic fracturing operations for shale gas in Lancashire (UK) were stopped after earthquakes were 80 triggered by fluid injection (Clarke et al., 2019). Triggered felt seismicity has already been reported at the 81 United Downs deep geothermal pilot in Cornwall (Holmgren & Werner, 2021). Note that, in both of these 82 cases, fracturing and/or fault slip are intrinsic to the success of the operation as they are needed to enhance 83 fluid flow, and therefore earthquakes are inevitable. In detail, microseismicity (i.e., M<2) is inevitable, but it 84 is important to understand whether felt (i.e. M>2) seismicity can be forecast ahead of time. Furthermore, 85 many sites for energy transition projects in the UK are located in (beneath) areas of extreme poverty and 86 social deprivation, both rural (e.g., Cornwall, South Wales) and urban (e.g., Greater Manchester, Glasgow), 87 and therefore the risks from these projects fall disproportionately on the less well off (Nolan, 2016; 88 McLennan et al., 2019). To begin to address these complex issues, we need to quantify which faults are more 89 or less likely to slip in response to induced changes in loading. One approach is to analyse data during 90 subsurface operations and attempt to manage the consequences (e.g., Verdon & Budge, 2018). An 91 alternative approach, and the one taken in this paper, is to look at the bigger picture before operations 92 commence and reduce risk from the outset.

93 Various measures have been proposed to quantify the propensity or tendency of a given fault to slip (or 94 open) in a known stress field. The following methods are based around an assumption of Mohr-Coulomb 95 (brittle-plastic) failure which has been shown to capture the key aspects of faulting in the upper crust. Slip 96 tendency (*T*_s) was introduced by Morris et al. (1996) and is the simplest measure of fault stability, defined as:

97
$$T_s = \tau / \sigma_n$$

98 where τ is the shear stress and σ_n is the normal stress acting on the fault plane. These stress components in 99 turn depend on the principal stresses and the orientation of the fault plane (see Lisle & Srivastava, 2004 for 100 details). In the absence of cohesion, if the slip tendency on a fault equals or exceeds the coefficient of sliding 101 friction, then the fault can be deemed "unstable". This dimensionless index embodies the key mechanical

(1)

principle underlying Mohr-Coulomb shear failure: as the shear ("sliding") stress acting on a fault plane rises
 in relation to the normal (or "clamping") stress, the fault approaches failure and will slip. Dilation tendency
 (T_d) has been defined to describe the propensity for a fault to open, or dilate, in a given stress regime:

105
$$T_d = (\sigma_1 - \sigma_n)/(\sigma_1 - \sigma_3)$$
(2)

where σ_1 and σ_3 are the principal stresses of the *in situ* stress tensor (Ferrill et al., 1999).

107 Most rocks in the upper crust are porous and permeable to some degree, and fault rocks are no exception, 108 so these rocks are generally fluid saturated. This implies that we should include pore fluid pressure and the 109 concept of effective stress in our assessment of fault stability. Fracture susceptibility (*S*_f) is the change in pore 110 fluid pressure needed to push a stressed fault to failure (Streit & Hillis, 2004) and is defined by:

111
$$S_f = \Delta P_f = (\sigma_n - P_f) - (\tau - C_0)/\mu$$
(3)

where P_f is the pore fluid pressure at the fault, C_0 is the cohesive strength (or cohesion), and μ is the coefficient of sliding friction (see Figure 1b).



114

115 Figure 1. a. Schematic block diagram of a fault plane showing the terminology used in this paper. Also shown are the cartesian and geographic reference frames and the Andersonian principal stresses. b. Mohr diagram 116 117 for a given state of stress (blue semi-circle) with normal (σ_n) and shear stresses (τ) marked for a selected fault 118 plane orientation (blue dot). Failure envelope for frictional sliding (cohesion=0) also shown as straight blue 119 line. c. Mohr diagram depicting one of the key issues tackled in this paper: given uncertainty in the input 120 stress values (grey Mohr circles for the variation around the average principal stresses in red, blue and green), 121 what is the probability of failure? i.e., what percentage of all these stress states will intersect the failure 122 envelope?

123 Previous applications of these three measures of fault stability $-T_s$, T_d and S_f - cover the full spectrum of rock 124 types and stress fields, from basins to basement and from extensional, contractional and wrench tectonic 125 settings. Applications within the domain of the energy transition include examples from geothermal energy 126 (both shallow and deep) and CCS. The original definition of fracture susceptibility by Streit & Hillis (2004) was 127 concerned with safe injection limits for CO2 in potential reservoirs in Australia. Moeck et al. (2009) used slip 128 tendency to quantify the relative stability of different fault sets in different horizons in a geothermal reservoir 129 in the North German Basin, and Barcelona et al. (2019) used a similar method for Copahue geothermal 130 reservoir in Argentina. For CCS, Williams et al., (2016, 2018) have used slip tendency analyses of faults in 131 potential sandstone reservoirs on the UK continental shelf, including the North Sea and East Irish Sea basins. 132 The links between subsurface fluid flow, seismicity, and fault stability have recently been explored by Das &

- 133 Mallik (2020) for the Koyna earthquakes in India, and by Wang et al. (2020) for strike-slip faults in the Tarim
- 134 Basin of China.

135 Probabilistic approaches to fault stability have been adopted by various workers. In risking CO₂ storage for 136 an oil reservoir in the Williston basin, Ayash et al. (2009) used a features, events and processes (FEP) 137 approach to constrain the likelihood of occurrence of fault slip (based on slip tendency) and the severity of 138 the consequences, with their product defined as the risk. Rohmer & Bouc (2010) used RSM to assess cap rock 139 integrity for tensile or shear failure above deep aquifers in the Paris basin targeted for the storage of CO2. 140 Coupled RSM and Monte Carlo approaches to fault stability have been used by Chiaramonte et al. (2008) and 141 Walsh & Zoback (2016), following their initial application in the field of wellbore stability by Moos et al. 142 (2003). This Fault Slip Potential (FSP) method developed by Stanford (e.g., Chiaramonte et al., 2008 & Walsh 143 & Zoback, 2016) calculates the response surface for fracture susceptibility, with the in situ stress tensor 144 calculated by inversion of abundant seismicity data (focal mechanisms), and then uses a Monte Carlo 145 simulation to generate cumulative distribution functions (CDFs) of conditional probability of slip defined with 146 reference to an arbitrary pore pressure perturbation ($\Delta P_f = 2$ MPa, in the case of Walsh & Zoback, 2016). 147 Note that FSP assumes cohesionless faults ($C_0=0$) and hydrostatic pore fluid pressure, and that conditional 148 probability in this sense refers to the fact that we do not know where any particular fault is with respect to 149 the seismic cycle.

150 Conventions and layout for this paper

151 In the sections below, we describe the underlying equations for measuring fault stability and then show how 152 we can use Response Surface Methodology (RSM) from engineering to explore the consequences of 153 uncertainties in the input variables. After assessing the quality of the solutions obtained from RSM, we then 154 apply a brute force Monte Carlo (MC) approach to generate cumulative distribution functions (CDFs) of the 155 different measures (T_s , T_d and S_f). The case studies use published, publicly available data to constrain the 156 input variable distributions and then a combined RSM/MC approach is used to explore the uncertainty in 157 fault stability in different settings.

158 In this paper, compressive stress is reckoned positive, with σ_1 as the maximum compressive principal stress 159 and σ_3 as the minimum principal stress. Stress states and fault regimes are assumed to be Andersonian, with 160 one principal stress vertical, although the underlying model and code could be changed to incorporate non-161 Andersonian stress states with the addition of extra variables for the stress tensor orientation (Walsh & 162 Zoback, 2016). The likelihood of slip on a fault is assessed in the framework of Mohr-Coulomb failure, with or without cohesion (Jaeger et al., 2009). Fault orientations are quantified as strike and dip, following the 163 right-hand rule: with your right hand flat on the fault plane and fingers pointing down dip, the right thumb 164 165 points in the direction (azimuth) of strike. The relationship between the geographical and cartesian reference 166 frames follows a North-East-Down convention. Figure 1 depicts the key terms and elements used in the 167 analysis, and Table 1 contains a list of terms and symbols used with units where appropriate.

Quantity	Symbol	Units
Maximum compressive stress	σ_1	MPa
Intermediate compressive stress	σ_2	MPa
Minimum compressive stress	σ_3	MPa
Vertical stress	σ_V	MPa
Maximum horizontal stress	σ_{Hmax}	MPa
Minimum horizontal stress	σ_{hmin}	MPa
Azimuth of max. horizontal stress	sHaz	0
Pore fluid pressure	P_f	MPa
Coefficient of friction	μ	dimensionless
Cohesive strength (or cohesion)	Co	MPa
Slip tendency	Ts	dimensionless
Dilation tendency	T _d	dimensionless
Fracture susceptibility	S _f	MPa
Fault strike	φ	0

Fault dip	δ	0
Shear stress on a fault plane	τ	MPa
Normal stress on a fault plane	σ_n	MPa

- **Table 1.** List of terms and symbols used in this paper, with units where appropriate.
- 170

171 Statistical analysis of geomechanical fault stability

172 Introduction to Response Surface Methodology (RSM)

173 RSM is widely used in engineering and industry along with a Design of Experiments approach, and often 174 employed to optimise a specific process of interest – e.g., to maximise the yield of a reaction given the input 175 variables of pressure, temperature, reactant mass etc. RSM is a large and growing field and is best considered 176 as a toolbox of different methods with a common mathematical basis. The governing equations for RSM were 177 derived by Box & Wilson (1951). The core idea is that a response y can be represented by a polynomial 178 function of a number (q) of input variables $x_1 - x_q$:

179
$$y = f(x_1, x_2, \dots, x_n)$$
 (4)

Each of the *q* input variables can be represented by either a discrete set of measurements made in the
laboratory (or field) or drawn from appropriate statistical distributions (normal/Gaussian, skewed normal,
Von Mises etc.). The simplest polynomial function that relates *y* and *x* is a linear one:

183
$$y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \dots + \beta_q x_{Nq} + \epsilon_i$$
 (5)

 $y_i = \beta_0 + \sum_{i=1}^q \beta_i x_{ii} + \epsilon_i$

185 where
$$\beta_q$$
 are the coefficients (to be determined), y_i is the set of observations of the response ($i = 1, 2, ..., N$),
186 and x_{ij} are the input variables ($j = 1, 2, ..., q$). ϵ is the experimental error, and the number of 'observations' N
187 > q , the number of input variables. This is therefore a multiple regression model linking the response y to

(6)

188 more than one (i.e., multiple) independent variables, *x*.

189 A more complex polynomial relationship is the quadratic form:

190

$$y = \beta_0 + \sum_{j=1}^{q} \beta_j x_j + \sum_{j=1}^{q} \beta_{jj} x_j^2 + \sum_{i< j}^{q} \beta_{ij} x_i x_j + \epsilon$$
(7)

191 This 2nd order multiple regression model contains all the terms of the linear (1st order) model, but also extra 192 terms for the squares and cross-products of the input variables (second and third terms on the RHS of 193 equation 7).

194 To define a response surface, either linear or quadratic, we need to calculate the values of the β_q coefficients. 195 We can rewrite the key equations in matrix form:

196

$$y = X\beta + \epsilon \tag{8}$$

where **y** is an (N x 1) vector of observations (or calculations), **X** is an (N x k) matrix of input variable values (k = q + 1), and β is a (k x 1) vector of regression coefficients. We solve this system of equations using the standard linear algebra technique of least squares regression (Myers et al., 2016):

 $\widehat{\boldsymbol{\beta}} = (\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{X}'\boldsymbol{y} \tag{9}$

201 The response surface (linear or quadratic) is then defined by

 $\widehat{y} = X\widehat{\beta} \tag{10}$

The values used in **X** are chosen to efficiently span the parameter space. A typical sampling design for **X** is called the 3^q model with 3 values of each variable, usually the minimum, mean (or mode) and maximum. For slip tendency, q = 6 and this means we use $3^q = 3^6 = 729$ data points to calculate the response surface. In practice, coded variables are used in **X** where the absolute values for the minimum, mean and maximum of each variable are scaled to -1, 0 and +1 respectively, and then scaled back when the response surface is used in the Monte Carlo simulation (Myers et al., 2016).

The response surface – i.e., the set of β coefficients – is defined using a limited number of sample points, depending on the chosen sample design (3^{*q*} in the examples used in this paper; other variants exist – see Myers et al., 2016 for details). To explore the possible variations of a response more fully, we use a Monte Carlo (MC) approach of pre-defined size (N_{MC} = 5,000 in the examples in this paper). The MC simulation uses the response surface calculated from the design points to calculate the responses for N_{MC} combinations of input variables drawn from their distributions. This produces a statistically viable ensemble of response values from which we can infer the probability of the response with respect to a chosen threshold.

216 With respect to fault stability, we can use RSM to produce a parameterised relationship – the response 217 surface in q dimensions – between a stability measure of interest and the q input variables. In the case of slip 218 tendency T_s , we can rewrite the components of equation 1 in terms of the measurable input quantities as 219 follows:

(12)

220
$$\tau = \sqrt{(\sigma_1 - \sigma_2)^2 l^2 m^2 + (\sigma_2 - \sigma_3)^2 m^2 n^2 + (\sigma_3 - \sigma_1)^2 l^2 n^2}$$
(11)

$$\sigma_n = \sigma_1 l^2 + \sigma_2 m^2 + \sigma_3 n^2$$

where *I*, *m* and *n* are the direction cosines of the normal (pole) to the fault plane given by

223 $l = \sin \delta \sin \phi$ (13a)

$$m = -\sin\delta\cos\phi \tag{13b}$$

$$225 n = \cos \delta (13c)$$

where ϕ is the fault strike and δ is the fault dip, in a North-East-Down reference frame (Allmendinger et al., 2012).

228 All terms on the right-hand sides of equations 11-13 are uncertain to some degree, therefore estimating the 229 uncertainty of T_s , and as importantly, the key controls on the uncertainty of T_s , in terms of these input 230 variables, is non-trivial. This difficulty in estimating and visualising possible variations in our estimates of T_s 231 is exacerbated by the recognition that each of the input variables may be distributed differently: some 232 quantities (e.g., the principal stresses) may follow normal (Gaussian) statistics, whereas others (e.g., strike, 233 dip, sHmax azimuth) will follow Von Mises distributions. In the case of fracture susceptibility (S_{f} , equation 3), 234 it is even more complicated with the addition of three further input variables for friction, cohesion and pore 235 fluid pressure. Measurements or calculations of coefficients of friction and cohesive strength often display 236 asymmetric or skewed distributions (skewed high or low), and this adds further complexity to the task of 237 estimating and constraining fault stability from the data at hand.

238 Worked Example 1: Slip tendency from synthetic input data

The calculations presented in this paper were all performed with the custom pfs (**p**robability of **f**ault **s**lip) package, written by the first author (DH) in Python 3, and freely available on GitHub (see Code Availability, below).

The first example calculates a response surface for slip tendency (T_s) from q=6 input variables: the magnitudes of the three principal stresses of the *in situ* stress tensor (σ_1 , σ_2 , σ_3) assumed Andersonian with one principal stress vertical, the azimuth of the maximum horizontal stress (*sHaz*), and the strike and dip of the fault plane. This response surface is then used in a Monte Carlo simulation (N_{MC} = 5,000) to generate a CDF of T_s values for the fault. The specific Python code to run this example in the pfs package is wrapped in a Jupyter notebook available on GitHub (WorkedExample1.ipynb).

The first task is to define the distributions of the input variables. In pfs, examples are shown for normal, skewed normal and Von Mises (circular normal) distributions, but other statistical distributions are allowed.

250 Table 2 and Figure 2 describe the ranges and moments of these distributions for each input variable. For this

example, the normally distributed principal stresses are defined with a variation (standard deviation) of 5% of their central (mean) value, and the Von Mises distributions of the azimuthal variables (sHaz, strike and dip) all have $\kappa = 200$ to model their dispersion about their mean. The fault of interest strikes 060° and dips 60° to

- the south (right hand rule). The key questions to be addressed by this example are:
- 255 1. given these uncertainties in the input stresses and orientation data, how does the estimation of T_s 256 vary? What is the range and the mode?
- 257 2. which variables exert the greatest (and least) control on the predicted variation in T_s ?

258 We first build a response surface using a 3^q design, i.e., 3 data points for each variable – minimum, mean and 259 maximum – and for $T_{s_r} q = 6$. This means we calculate the response surface from $3^6 = 729$ data points. We 260 compare a calculated linear response surface with a quadratic response surface, using a normal probability 261 plot of residuals (Figure 3). These residuals are the differences between the values of T_s derived from the 262 observations (taken from the input distributions shown in Table 2 (upper) and Figure 2), and the calculated 263 values of T_s using the β coefficients derived by least squares regression i.e., the response surface. The 264 adjusted R^2 value for the quadratic 2nd order model is significantly better than that for a linear 1st order model, 265 and we use quadratic models throughout the rest of this paper. More detailed inspection of the quality of fit between the response surface and the observations is possible, including analysis of variance, main effects 266 267 plots and the use of t-statistics for each input variable to quantify their significance to the definition of the β 268 coefficients (Myers et al., 2016). In practice, visualising sections of the response surface for individual 269 variables is generally sufficient (see below; Moos et al., 2003; Walsh & Zoback, 2016).

Variable	Mean	Standard deviation	Units	Distribution	Comments	
		(<i>ĸ</i> for Von Mises)				
Worked Example 1 – Synthetic T _s – modelled depth=3 km						
σ_v , vertical stress	75.0	3.75	MPa	Normal	Lithostatic for depth	
		(5% of mean)			of 3 km, assuming	
					average rock density	
					of 2500 kg m ⁻³	
σ_{H} , max. horizontal	50.0	2.5	MPa	Normal	Andersonian normal	
stress		(5% of mean)			faulting regime	
σ_h , min. horizontal	25.0	1.25	MPa	Normal		
stress		(5% of mean)				
Azimuth of σ_{Hmax}	060	к=200	o	Von Mises		
				(circular		
				Normal)		
Fault strike	060	к=200	o	Von Mises		
				(circular		
				Normal)		
Fault dip	60.0	<i>к</i> =200	0	Von Mises		
				(circular		
				Normal),		
				truncated at 0		
				and 90		
	Worked Example 2 – Synthetic S _f – modelled depth=3 km					
σ_v , vertical stress	75.0	7.5	MPa	Normal	Lithostatic for depth	
		(10% of mean)			of 3 km, assuming	
					average rock density	
					of 2500 kg m ⁻³	
σ_{H} , max. horizontal	55.0	5.5	MPa	Normal		
stress		(10% of mean)				
σ_h , min. horizontal	35.0	3.5	MPa	Normal		
stress		(10% of mean)				

<i>P</i> _f , pore fluid pressure	30.0	3.0 (10% of mean)	MPa	Normal	Hydrostatic for depth of 3 km, assuming fluid density=1000 kg m ⁻³
Azimuth of σ_{Hmax}	060	<i>к</i> =200	o	Von Mises (circular Normal)	,
Fault strike	060	<i>к</i> =200	o	Von Mises (circular Normal)	
Fault dip	60.0	<i>к</i> =200	o	Von Mises (circular Normal), truncated at 0 and 90	
Friction, μ	0.6	0.12 (20% of mean)	n/a	Skewed normal	$\alpha = -3$
Cohesion, C ₀	20.0	2.0 (10% of mean)	MPa	Skewed normal	$\alpha = +3$ i.e., skewed high

Table 2. Table of input variable distributions for the synthetic models in Worked Examples 1 and 2.



272

Figure 2. Histograms of input variables used to calculate slip tendency T_s for the synthetic distributions shown in Table 2.



Figure 3. Residual plots for linear and quadratic response surfaces for slip tendency using synthetic data. The
 quadratic fit has a higher value of the adjusted R² parameter and is therefore deemed better in this case.

Having generated the quadratic response surface for T_s for these input distributions, we can now use it to perform a Monte Carlo (MC) simulation with the aim of generating a statistically viable ensemble from which we can infer the probability of T_s exceeding a critical value of sliding friction. The results from the MC analysis of T_s are shown in Figure 4. The histogram of all values of T_s shows a symmetrical and rather narrow distribution with a modal value of about 0.56 (Figure 4a). The CDF of all values of T_s also shows this narrow and symmetrical distribution (Figure 4b).

284 A response surface of more than two variables is not easy to visualise. One approach is to take sections 285 through the surface at specific values of all but one variable and graph that. The red lines shown in Figure 2 286 depict the response surface for that variable with all other variables held at their mean values. Thus the red 287 line in Figure 2a shows the variation in T_s as σ_1 varies with all other variables (σ_2 , σ_3 , sHaz, φ and δ) held at 288 their mean values. There is a clear positive correlation of increasing T_s with increasing σ_{I} , as expected from 289 the definition of T_s and its underlying dependence on differential stress (= $\sigma_1 - \sigma_3$); the clear negative 290 correlation of T_s with σ_3 shown in Figure 2c confirms this. Many of the response surface sections shown in 291 Figure 2 are quasi-linear, but some are not: in particular, the dependencies of T_s on sHaz, strike and dip are all non-linear, and this further justifies the selection of a 2nd order quadratic response surface model. 292

293 A useful way to visualise the results from the response surface calculated by the MC simulation is the tornado 294 plot shown in Figure 4c. Here the ranges of T_s for each input variable (shown as red lines over the histograms 295 in Figure 2) are plotted to show the relative sensitivity of T_s to each variable. Variables are ranked from the 296 largest range at the top to the lowest range at the bottom. Again, the core dependence of T_s on differential 297 stress (= $\sigma_1 - \sigma_3$) is apparent, with σ_1 and σ_3 ranked highest in the plot. Interestingly, fault dip is ranked the 298 next highest in terms of sensitivity and this reflects the geometry of this particular example. The Andersonian 299 stress regime is for normal faulting, with σ_1 vertical. σ_2 is oriented parallel to fault strike (sHaz = strike = 060), 300 and the fault dips at 60. This fault is therefore ideally oriented for slip in this stress field. Small changes to dip 301 will influence the ratio of τ to σ_n , and therefore T_s .



275

Figure 4. Output from Monte Carlo simulation (N_{MC} =5,000) of slip tendency calculated using a quadratic response surface from synthetic input data. **a**. Histogram of calculated slip tendency values, in this case showing a quasi-normal distribution with a mode of ~0.55. **b**. Cumulative distribution function (CDF) of calculated slip tendency values, showing the range in values from ~0.4 to ~0.7. **c**. Tornado plot showing relative sensitivity to the input variables. The vertical dashed line shows the modal (most frequent) value of T_s from the MC ensemble.



309

Figure 5. Output from Monte Carlo sensitivity tests for slip tendency, T_s . **a**. Effect of variation in standard deviation of the least principal stress, σ_3 . **b**. Effect of variation in dispersion (κ parameter of the Von Mises distribution) of fault dip.

313 We can use a Monte Carlo approach to explore these sensitivities in more detail. Given the shape of the 314 response surface sections shown in Figure 2 and the ranking of variables in Figure 4c, we can quantify how 315 more or less variation in the inputs will affect the predicted T_{s} . Figure 5 shows the results of this sensitivity 316 analysis for σ_3 and fault dip. The most significant effect on the CDF of T_s is produced by increasing the 317 variation in σ_3 to 20% of the mean. This level of uncertainty for the minimum stress is not unreasonable in 318 real-world scenarios (see Case Studies below). Increased uncertainty in σ_3 at this level leads to a ~20% chance 319 of T_s being in excess of 0.7 (p = 0.8 for $T_s \le 0.7$ from Figure 5a). Increased uncertainty in fault dip is achieved by varying the dispersion parameter κ of the Von Mises distribution (lower values of κ = more dispersed). 320 321 Very disperse distributions of fault dip with κ = 20 only change T_s by < 0.1.

322 Worked Example 2: synthetic Sf

We can explore variations in predicted fracture susceptibility using the same principles as for slip tendency, but adjusted by incorporating three new variables as required by equation 3 - pore fluid pressure, friction coefficient and cohesion (code in GitHub: WorkedExample2.ipynb). The number of variables *q* is now 9, and therefore the design space used to compute the response surface is $3^q = 3^9 = 19,683$ data points. In practice this means a slower run-time, but still only takes a few minutes on a modern processor.

For this example, we use the same stress tensor as for the T_s example, with σ_1 as the maximum principal stress and vertical, i.e., an Andersonian normal fault regime for a depth of approximately 3 km. We constrain

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330 the in situ pore pressure with a symmetrical normal distribution with a mean value of 30 MPa, which is approximately hydrostatic for a depth of 3 km, and with a variation of 10% of this mean. Friction is 331 332 constrained by a skewed normal distribution with a mode of 0.56 and $\alpha = -3$, i.e., skewed towards lower 333 values. This shape of distribution for friction coefficients is consistent with previous studies (e.g., Moos et al., 334 2003; Walsh & Zoback, 2016) but is open to question (see Discussion). Similarly for cohesion, we use a skewed 335 normal distribution with a mode of 21 MPa and α = +3, i.e., skewed towards higher values again consistent 336 with previous work. These input variable distributions are documented in Table 2 (lower) and shown in the 337 histograms of Figure 6.





Figure 6. Histograms of the input variables, in addition to those shown in Figure 2, used to calculate fracture susceptibility for the synthetic distributions shown in Table 2. Note the skewed (asymmetric) distributions

341 for μ and C_0 .



342

Figure 7. Output from Monte Carlo simulation (N_{MC} =5,000) of fracture susceptibility calculated using a quadratic response surface from synthetic input data. **a**. Histogram of calculated fracture susceptibility, showing a quasi-normal distribution with a mode of 21.7 MPa. **b**. Cumulative distribution function (CDF) of calculated fracture susceptibility, showing the range in values from just less than 0 to about 60 MPa. **c**. Tornado plot of relative sensitivities of the input variables used to calculate fracture susceptibility.

348 We calculate a quadratic response surface and use a Monte Carlo simulation (N_{MC} = 5,000) to generate the 349 ensemble summarised in Figure 7. The mode of the distribution of S_f is 21.7 MPa meaning that, on average, 350 an increase in pore fluid pressure of about 22 MPa above the average in situ value of 30 MPa is needed to 351 push the effective stress state to Mohr-Coulomb failure. The histogram in Figure 7a is approximately 352 symmetrical, perhaps with a slight skewness to higher values, and this is reflected in the CDF shown in Figure 353 7b. The distribution is overwhelmingly positive, meaning that this fault is almost unconditionally stable for 354 any change in pore fluid pressure, at these conditions. The response surface sections for μ , C_0 and P_f shown 355 in Figure 6 (red lines) all show a strong influence on the fracture susceptibility, and these are confirmed in 356 the tornado plot of Figure 7c. Pore fluid pressure exhibits a negative correlation with S_f (Figure 6c) which is 357 consistent with the general principle of effective stress: i.e., if the original in situ pore pressure is already

- high, it only takes a small perturbation (small $\Delta P_f = S_f$) to promote sliding failure. The response to changes in
- 359 μ and C_0 is more interesting (Figure 6a and b). For this magnitude of cohesion, the effect of cohesion on S_f is
- 360 greater than that of μ (C_0 ranks higher than μ in the tornado plot, Figure 7c), and the dependence of S_f on μ
- is negative. However, this relationship is not general as will be shown in the Case Study for the PorthtowanFault Zone (see below).



Figure 8. Sensitivity of fracture susceptibility to variations in μ and C_0 . Note the changes in scale along the xaxis between the plots.

The relative asymmetries of the skewed normal distributions for μ and C_0 have already been noted. Given 366 their significant effect on S_f (high ranking in the tornado plot, Figure 7c), it is useful to explore how the 367 368 skewness of these distributions might influence Sf. Figure 8 shows the results of repeated Monte Carlo 369 sensitivity tests for μ (Figure 8a, b) and C_0 (Figure 8c, d). For friction, a positive skewness to higher values (α > 0) would tend to reduce S_f – i.e., faults would be less stable. For cohesion, the opposite is true – a negative 370 skewness (α < 0) would make faults less stable to changes in P_f. These asymmetries are opposite to the ones 371 372 used in the main Worked Example 2 and used by other workers (see Discussion). Widening the distributions 373 for μ or C_0 by increasing their standard deviations (and retaining the original α values) tends to broaden the 374 distribution of predicted S_f with asymmetry to higher (i.e., more stable) values.

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376 Case Studies

The case studies have been chosen to illustrate how a combined RSM/MC approach can be used to estimate 377 the probability of slip on one or more faults, and to show that even with relatively good - i.e., complete -378 379 input data, these predictions highlight that industrial operations remain significantly hazardous, with a greater than 1 in 3 chance of slip on many faults across different settings. Selected specific aspects of the 380 381 modelling and the visualisation of results are emphasised in each case study. Figure 9 shows a map of the UK with the case study areas marked, together with the locations of instrumentally-recorded earthquakes and 382 383 their focal mechanisms (Baptie, 2010). Also shown are data from the World Stress Map database of 2016 384 (Heidbach et al., 2018) indicating the orientation of the maximum horizontal stress. A basic observation from 385 this map is the level of complexity and heterogeneity in the present day seismotectonics of the UK, reflecting the variation in the subsurface geology. However, there is a broad prevalence of NW-SE trending σ_{Hmax} directions and strike-slip earthquake mechanisms.



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Figure 9. Map of most of the UK showing the locations of the selected case studies. Also shown: epicentres
 of seismicity (light blue dots; BGS catalogue – Musson, 1996), focal mechanisms (blue and white; Baptie,
 2010), and orientations of the maximum horizontal stress (black lines; World Stress Map data – Heidbach et
 al., 2018).

393 1. Porthtowan Fault Zone in Cornwall, UK

The Porthtowan Fault Zone (PFZ) cuts the Carnmenellis granite in Cornwall in southwest England (Figure 10). This granite is a target for deep high-enthalpy geothermal energy due to its high radiogenic heat production (Beamish & Busby, 2016). Following the Hot Dry Rock (HDR) project in the 1980s (Pine & Batchelor, 1984; Batchelor & Pine, 1986), the United Downs pilot project has drilled two boreholes (UD-1, UD-2) to intersect the fault zone at depths of about 5,275 m and 2,393 metres, respectively, making UD-1 the deepest onshore borehole in the UK. The pilot project relies on shear-enhanced stimulation of pre-existing fractures (joints, 400 partially filled veins and faults) to drive fluid flow from the shallow injector (UD-2) to the deeper producer

401 (UD-1). Temperatures at the base of UD-1 have been predicted at about 200°C (Ledingham et al., 2019).

402 Shearing and downward flow of injected fluid was observed in boreholes as part of the earlier HDR project

403 and tracked with measured microseismicity (Pine & Batchelor, 1984; Green et al., 1988; Li et al., 2018).



404

Figure 10. Map of South West England showing: selected population centres, the United Downs deep geothermal pilot project and the former Hot Dry Rock project (black squares); epicentres of seismicity (light blue dots; BGS catalogue – Musson, 1996); focal mechanisms (blue and white; Baptie, 2010); and orientations of the maximum horizontal stress (black lines; World Stress Map data – Heidbach et al., 2018). Approximate trend and extent of the Porthtowan Fault Zone shown in pale red. Inset shows an equal area rose diagram with strikes of fault segments in the Porthtowan Fault Zone measured on BGS Falmouth sheet 352 (*N*=140; circular mean strike=158°, circular standard deviation=27°).

Figure 10 shows a map of SW England overlain with seismicity data from the BGS (Musson, 1996). The PFZ is poorly exposed inland, and runs NNW-SSE from Porthtowan on the north Cornish coast to Falmouth on the south coast (see inset rose diagram for strikes of constituent faults taken from the BGS Falmouth sheet 352). Overall, the fault zone is believed to dip steeply to the east at around 80° (Fellgett & Haslam, 2021). The azimuth of the maximum horizontal stress is broadly NW-SE, with one exception trending NE-SW.



418 Figure 11. a. Red triangles show Raspberry Shake (network code: AM) and BGS (network code: GB) seismic 419 stations in Cornwall, with station names labelled. Seismicity during geothermal operations is indicated by red 420 circles. The inset shows a close-up of the area demarcated by the blue dashed line in the main map. The black dashed line in the inset shows the broad WNW-ESE alignment in seismicity. **b**. Computed focal mechanism 421 422 for the 2020-09-30 11:44:01 M_L 1.6 induced earthquake. First-motions are plotted on the focal sphere with "+" indicating positive polarity, and "o" for negative polarities. P-wave first-motions are plotted starting and 423 424 ending 0.3 seconds before and after the picked arrival, respectively, and are coloured in the same way as the 425 points on the focal sphere.

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Figure 12. Constraints on input variables for the Porthtowan Fault Zone modelling. **a**. Stress-depth plot based on data and equations from the Hot Dry Rock project in the Carnmenellis granite (Batchelor & Pine, 1986). Also shown are the depths of the two wells in the pilot project at United Downs. **b**. Mohr diagram showing data from laboratory mechanical tests of Zhao (1987) for brittle failure of Carnmenellis granite at 200°C. Estimated Mohr-Coulomb failure envelope (dashed red line) is defined by μ =0.85, C_0 =30 MPa.

433 Detailed geomechanical analyses were performed in the Carnmenellis granite in the 1980s as part of the HDR 434 project, and these provide useful constraints on the variation of stress and fluid pressure with depth (Figure 435 12a; Batchelor & Pine, 1986). From these data, a strike-slip regime is most likely with $\sigma_1 = \sigma_{Hmax}$ and $\sigma_2 = \sigma_V$, 436 but note the uncertainties (based on quoted values in Batchelor & Pine, 1986): from around the depth of the 437 injector well at United Downs and deeper, a normal fault regime is also consistent with the data, i.e., $\sigma_1 = \sigma_V$ 438 and $\sigma_2 = \sigma_{Hmax}$. Note that the earlier HDR project did not target a specific fault zone in the granite.

The thermo-mechanical properties of the Carnmenellis granite have been studied by Zhao (1987). Figure 12b shows a Mohr diagram of data taken from Table 2.3 of Zhao (1987) for laboratory brittle failure tests conducted at 200°C (the approximate temperature of the injector well at United Downs). From these data, we have estimated a linear Mohr-Coulomb failure envelope defined by a friction coefficient of 0.85 and a 443 cohesive strength of 30 MPa. At the time of writing there are no published data for the mechanical properties444 of fault rocks sampled from the Porthtowan Fault Zone in the Carnmenellis granite.

We present model results for fracture susceptibility in the PFZ as the plan at United Downs (and elsewhere in the future) is to inject fluid into the fault zone in order to generate shear-enhanced permeability on preexisting fractures. Table 3 lists the input variable distributions used in the "base case" model for hydrostatic pore fluid pressure in the fault zone and mechanical properties taken from laboratory tests of intact Carnmenellis granite (Figure 12b). The modelled depth is chosen as 4 km, in between the depths of the UD-

450 1 and UD-2 wells.

Variable	Mean	Standard deviation	Units	Distribution	Comments
		(<i>ĸ</i> for Von Mises)			
σ_v , vertical stress	105.0	5.25	MPa	Normal	Lithostatic for depth
		(5% of mean)			of 4 km, assuming
					average rock density
					of 2650 kg m ⁻³
					Batchelor & Pine, 1986
σ _н , max.	125.0	25.0	MPa	Normal	Batchelor & Pine, 1986
horizontal stress		(20% of mean)			
σ_{h} , min. horizontal	53.0	5.3	MPa	Normal	Batchelor & Pine, 1986
stress		(10% of mean)			
<i>P_f</i> , pore fluid	40.0	4.0	MPa	Normal	Hydrostatic for depth
pressure		(10% of mean)			of 4 km, assuming
					average fluid density
					of 1000 kg m ⁻³
Azimuth of σ_{Hmax}	140	<i>к</i> =200	o	Von Mises	Batchelor & Pine, 1986
				(circular	
				Normal)	
Fault strike	340	к=150	o	As mapped	Digitised from BGS
					тар
Fault dip	80.0	к=1000	o	Von Mises	
				(circular	
				Normal),	
				truncated at	
				0 and 90	
Friction, μ	0.85	0.17	n/a	Skewed	α = -3
		(20% of mean)		normal	i.e., skewed low
Cohesion, Co	30.0	6.0	MPa	Skewed	α = +3
		(20% of mean)		normal	i.e., skewed high

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Table 3. Distributions of input variables used in the base case model of fracture susceptibility in the
 Porthtowan Fault Zone.



455 Figure 13. Outputs from the Monte Carlo simulation of fracture susceptibility in the Porthtowan Fault Zone. 456 a-d. The response surface for the base case, with friction and cohesion estimated from the laboratory failure 457 tests of Zhao (1987), predicts positive fracture susceptibility i.e., a stable fault zone. The tornado plot (d) 458 shows that for relatively high values of cohesion (mode of $C_0=30$ MPa in this case), the sensitivity to variations 459 in friction is slight. e-h. In contrast, the response surface for the 'weak fault' case, with reduced values of 460 friction and cohesion (mode of μ =0.3, mode of C₀=10 MPa), predicts fault zone instability i.e., overwhelmingly 461 negative values of $S_{\rm f}$. The effect of friction on these predictions is now very strong, as shown in the shape of 462 the response surface for μ (e) and in the ranking within the tornado plot (h).

The results from the Monte Carlo simulation of S_f for the PFZ are shown in Figure 13. For the base case, with hydrostatic pore fluid pressure and a 'strong fault' (mode of μ =0.85, mode of C_0 =30 MPa), the fault appears unconditionally stable for the modelled *in situ* stress variations. The CDF shows almost exclusively positive values of S_f up to about 60 MPa. Note that, for the input stress variations listed in Table 3, 22% of the MC simulations produced an Andersonian normal fault regime ($\sigma_1 = \sigma_V$), rather than a strike-slip ($\sigma_2 = \sigma_V$) regime.

468 232 microseismic events with hypocentre depths of 4-5 km were detected by the BGS during geothermal 469 testing operations in 2021-2022 (http://www.earthquakes.bgs.ac.uk/data/data_archive.html; last accessed 470 23 July 2021). The largest earthquake induced by geothermal operations during this period occurred on 2020-471 09-30 11:44:01, and had a local magnitude of <u>M</u>_L 1.6, and was felt by residents in the area. This event was 472 well-recorded on a network of single-component Raspberry Shake stations (e.g. Holmgren & Werner, 2021) 473 and a single station of the BGS permanent monitoring network (Figure 11a). These stations offer excellent 474 azimuthal coverage of the geothermal seismicity, with the closest station lying only 2 km away (AM.RAD67). 475 Since no focal mechanisms have yet been documented for these induced earthquakes, we used recorded P-476 wave first motions to compute a focal mechanism of the M_L 1.6 event using the method of Hardebeck & 477 Shearer (2002). Take-off angles were computed using a 1D seismic velocity model for the Cornwall area 478 (http://earthwise.bgs.ac.uk/index.php/OR/18/015 Table 4: Depth/crustal velocity models used in eart 479 hquake locations; last accessed 23 July 2021). The best-fitting focal mechanism (Figure 11b) indicates either 480 normal faulting on a WNW-ESE steeply-dipping plane or strike-slip faulting on a shallow-dipping plane NE-481 SW striking plane. Single event relocated epicentres reported by the BGS, which use arrivals from a local 482 dedicated microseismic monitoring array, show a NW-SE trend (Figure 11a), consistent with normal faulting 483 on a steeply east-dipping, WNW-ESE striking plane during this earthquake. Negative P-wave polarities were 484 recorded at AM.RAD67 for all M > 0 events, indicating that the same fault plane was reactivated during many 485 of the induced events. The inferred fault plane is sub-parallel to the interpreted strike of the Porthtowan 486 Fault Zone that is targeted by the geothermal testing. This observed normal faulting mechanism is consistent with our MC simulations (more than 1 in 5 of the predicted stress states were for normal faulting). 487

489 The response surface (green lines on Figure 13a-b) and the tornado plot of relative sensitivities of the input 490 variables (Figure 13d) shows a positive dependence of S_f on the cohesion, and that variations in friction are 491 relatively unimportant. If we reduce the strength of the modelled fault zone, by changing the input 492 distributions of μ and C_0 to lower values – but with the same shape and skewness – the situation changes. 493 The predicted fracture susceptibility is now much more strongly correlated with variations in friction, and 494 less so with variations in cohesion. This can be explained by looking at the underlying formula for S_f (equation 495 3), in particular the 2nd term on the RHS. If $C_0 > \tau$ then the numerator of this term can be negative, producing 496 a net positive term. However, if $C_0 < \tau$ and μ is small then this term is larger and negative. The important 497 point is that the probability distribution of S_f (compare Figure 13c and 13g) is controlled by the *relative* 498 magnitudes of μ and C_0 . In a weak fault zone, with low μ and low C_0 , the predictions are very sensitive to the 499 value of friction. In a strong fault, the effect of μ is less important. Thus, we need to know more about the relationship between μ and C_0 in fault rocks (see Discussion). 500

501 2. Coalfields in South Wales and Greater Manchester, UK

502 Scope exists to extract low enthalpy geothermal heat from disused coalmines in the UK (Farr et al., 2016), 503 using either open- or closed-loop technology. Possible sites include the South Wales and Greater Manchester 504 coalfields, where folded and faulted Coal Measures of Westphalian (upper Carboniferous) age have been 505 mined for centuries, up until the 1980s. Initial plans for shallow mine geothermal schemes include passive 506 dewatering which may not change the loading on faults by much. However, active dewatering schemes can 507 promote ingress of deeper ground water (Farr et al., 2021), and as this fluid flow must be driven by gradients 508 in fluid pressure, this could in turn lead to the instability of faults at depth. The models below are for a depth 509 of 2 km.

510 The locations and orientations of faults have been taken from published BGS maps. For the South Wales 511 coalfield (Figure 14a), we used the BGS Hydrogeology map of S Wales to map the traces of faults in the Coal 512 Measures (Westphalian), and BGS 1:50k solid geology sheets over the same area to collect data on fault dips. 513 For the Greater Manchester coalfield (Figure 14b), we used the BGS 1:50k solid geology sheets for Wigan, 514 Manchester and Glossop. Faults were traced onto scanned images of the maps in a graphics package (Affinity 515 Designer on an Apple iPad using an Apple Pencil). These fault trace maps were saved in Scalable Vector 516 Graphics (.SVG) format, after deleting the original scanned image layer of the geological map. The saved .SVG 517 files were read into FracPaQ (Healy et al., 2017) to quantify their orientation distributions (inset rose plots in 518 Figure 14a and b). The fault trace maps were then overlain on maps containing historical seismicity and 519 available focal mechanisms (from the public BGS catalogue; Musson, 1996) and the orientations of σ_{Hmax} 520 taken from the World Stress Map project (Heidbach et al., 2018).

521 In the South Wales coalfield 3,408 fault segments were traced, and the dominant trend is clearly NNW/SSE, 522 but with important (and long) fault zones running ENE-WSW, such as the Neath and Swansea Valley 523 Disturbances (Figure 14a). From cross sections, we measured 142 fault dips to help constrain the distribution 524 of friction coefficients in these rocks (Figure 15b-c; see below), corrected for vertical exaggeration on the 525 section line where necessary. Focal mechanisms in this area (n=4) suggest that NNW/SSE and N/S faults are 526 active in the current stress regime. Historical seismicity is widely, if unevenly, distributed with no obvious 527 direct correlation to the surface mapped fault traces. For example, there are areas of intense surface faulting 528 but no recorded historical seismicity, and vice versa – areas with abundant historical events but few mapped 529 faults.

530 Around Greater Manchester 3,453 faults were traced, and the dominant trend is NW/SE, but E/W faults are 531 also present (Figure 14b). From cross sections, we measured 89 faults to help constrain the distribution of 532 friction coefficients in these rocks (Figure 15d-e; see below). Historical seismicity is again widely, if unevenly, 533 distributed with few obvious direct correlations to the surface mapped fault traces. However, there was an 534 earthquake swarm in 2002-2003 which comprised more than 100 events, with a maximum local magnitude 535 of 3.9. Calculated focal depths were 1 - 3 km, although these have large uncertainties (Walker et al., 2003). 536 The World Stress Map database has the orientation of σ_{Hmax} trending WNW/ESE in this area (Figure 12b). 537 These observations suggest that faults oriented more nearly E/W are more likely to slip in the current stress 538 regime.

There are no published geomechanical analyses for the variation of stress with depth for either of these two areas. To constrain the depth dependence of stress, we have used larger scale syntheses of stress for onshore UK produced by the BGS (e.g., Kingdon et al., 2016; Fellgett et al., 2018). The stress-depth plot in Figure 15a has been constructed using the data shown in Fellgett et al. (2018), and shows that, in general, a strike-slip fault regime with $\sigma_1 = \sigma_{Hmax}$ is most likely. However, given the known uncertainties in the data, a normal fault regime ($\sigma_1 = \sigma_V$) cannot be ruled out, especially at depth. The azimuth of σ_{Hmax} is known to vary across the UK ranging from ~130 to ~170 (Baptie et al., 2010; Becker & Davenport, 2001).

546 Despite the economic and historical significance of the Coal Measures, there are no published datasets of 547 laboratory measured friction or cohesion for either intact rocks or their faulted equivalents (although data 548 may exist in proprietary company records). Data for specific units of interest does exist, e.g., for the 549 Oughtibridge Ganister, a seat earth in the Coal Measures (Rutter & Hadizadeh, 1991); and the Pennant Sandstone, a rare marine sandstone unit (Cuss et al., 2003; Hackston & Rutter, 2016), but a systematic 550 551 analysis of the volumetrically dominant sandstone, siltstone and mudstone formations is notably absent. 552 Instead, we use the measured dips of faults in the Coal Measures as a proxy for the coefficient of sliding 553 friction, using the relationship

554

 $\mu = 1/\tan(\pi - 2\beta)$ equation 14

555 where β is the angle between the fault plane and σ_1 at failure (Jaeger et al., 2009; Carvell et al., 2014). Such a calculation assumes Mohr-Coulomb failure and that the current dip of the fault is reasonably close to the 556 557 dip at failure in the post-Westphalian deformation of the coalfields. For measured fault dips < 45°, we assume 558 that σ_1 was horizontal (Andersonian thrust/reverse fault regime) and for fault dips >= 45° we assume σ_1 was 559 vertical (Andersonian normal fault regime). In practice, some of these faults probably originated as strike-slip 560 faults (i.e., with a sub-vertical dip and σ_2 vertical), and some of their dips have almost certainly been modified by compaction since their formation. However, this method of estimating the likely range of friction 561 coefficients from measured dips remains simple to apply and useful to first order, in the absence of better 562 563 data. From the dip data, the calculated friction coefficients vary between 0.0 and 6.0 for South Wales, and 564 between 0.35 and 2.0 for Greater Manchester (Figures 15c and e, respectively).



566 Figure 14. Maps of selected UK coalfields (suggested sites of shallow mine geothermal energy) showing: selected population centres (black squares); epicentres of seismicity (light blue dots; BGS catalogue -567 568 Musson, 1996); focal mechanisms (blue and white; Baptie, 2010); and orientations of the maximum 569 horizontal stress (black lines; World Stress Map data – Heidbach et al., 2018). Inset equal area rose diagrams show orientations of mapped faults. a. South Wales area. Faults in the Coal Measures taken from the BGS 570 571 Hydrogeological Map of South Wales (1:125k) (n=3,408), with a circular mean strike=156° and a circular standard deviation=65°. b. Greater Manchester area. Faults in the Coal Measures taken from the BGS 1:50k 572 573 sheets Wigan, Manchester and Glossop (n=3,453), with a circular mean strike=143° and a circular standard deviation=64°. 574

575 Based on the values of sliding friction calculated from measured fault dips across both coalfields a threshold 576 stability value of μ =0.3 is taken as a reasonable lower bound for faulted rock. This is the value used to 577 compare with predicted slip tendencies calculated for each fault. For $T_s > 0.3$, the fault is deemed unstable, 578 for $T_s <= 0.3$ it is stable.





Figure 15. Constraints on input variables for the coalfield modelling of slip tendency. **a**. Stress-depth plot based on data from onshore UK (after Fellgett et al., 2018). Also shown is the modelled depth of 2 km. **b-e**. Histograms of fault dips measured cross-sections on published BGS 1:50k maps of South Wales and Greater Manchester, and calculated values of friction coefficients derived from these dips assuming Mohr-Coulomb failure. Byerlee friction (μ =0.6-0.85) shown as shaded pink box. Modelled critical values of friction (μ =0.3) shown by red lines.

Variable	Mean	Standard deviation	Units	Distribution	Comments
		(κ for Von Mises)			
_		South Wales coalfield Ts	model, d	lepth=2 km	I
σ_v , vertical stress	50.0	3.75	MPa	Normal	Lithostatic for depth
		(5% of mean)			of 2 km, assuming
					average rock density
					of 2500 kg m ⁻³
σ _н , max.	70.0	14.0	MPa	Normal	After Fellgett et al.,
horizontal stress		(20% of mean)			2018
σ_h , min. horizontal	35.0	3.5	MPa	Normal	After Fellgett et al.,
stress		(10% of mean)			2018
Azimuth of σ_{Hmax}	160	к=200	0	Von Mises	After Fellgett et al.,
				(circular	2018; Baptie, 2010;
				Normal)	WSM, 2016
Fault strike	-	-	0	As mapped	Digitised from BGS
					Hydrogeology sheet
Fault dip	n/a	к=25	0	Von Mises	Fitted to data taken
				(circular	from cross-sections
				Normal),	on BGS 1:50k sheets
				truncated at 0	229-231, 247-249,
				and 90	263, 263
Greater Manchester coalfield Ts model, depth=2 km					
σ_v , vertical stress	50.0	7.5	MPa	Normal	Lithostatic for depth
		(5% of mean)			of 2 km, assuming
					average rock density
					of 2500 kg m ⁻³

σ _H , max.	70.0	14.0 (20% of moon)	MPa	Normal	After Fellgett et al.,
norizontal stress		(20% 01 mean)			2018
σ_h , min. horizontal	35.0	3.5	MPa	Normal	After Fellgett et al.,
stress		(10% of mean)			2018
Azimuth of σ_{Hmax}	145	к=200	0	Von Mises	After Fellgett et al.,
				(circular	2018; Baptie, 2010;
				Normal)	WSM, 2016
Fault strike	-	-	0	As mapped	Digitised from BGS
					1:50k sheets 84-86
Fault dip	60.0	к=200	0	Von Mises	Fitted to data taken
				(circular	from cross sections
				Normal),	on BGS 1:50k sheets
				truncated at 0	84-86
				and 90	

Table 4. Distributions of input variables used to model slip tendency in the coalfields of South Wales andGreater Manchester.

590 Predictions of conditional probability for fault slip have been calculated for all faults in both coalfields using 591 slip tendency as the chosen measure: in the absence of detailed pore fluid pressure constraints or estimates 592 of cohesive strength, it is hard to justify modelling the fracture susceptibility. Slip tendency provides a first 593 order estimate of fault stability. A quadratic response surface was constructed for each coalfield using the 594 full range of measured fault strikes and dips, and the input variable distributions listed in Table 4 and 595 constrained by the data in Figure 15. Monte Carlo simulations (N_{MC} =5,000) were run for each mapped fault 596 segment with the other input variables drawn from their respective distributions. Note that the principal 597 stresses used were the same for both coalfields, for a depth of 2 km (see Table 4), but the azimuth of sHmax 598 was varied to reflect the regional differences reported by other authors (Becker & Davenport, 2001; Baptie, 2010), and the recorded focal mechanisms. 599

600 Output CDFs for all faults in both coalfields are shown in Figure 16. For South Wales (N=3,408 faults), 601 approximately 46% of faults are predicted to have a 1 in 3 chance of being unstable (i.e., $T_s > 0.3$, shown in 602 red), and 42% of faults are predicted to have a 1 in 10 chance of being unstable (shown in amber). For Greater 603 Manchester (N=3,453 faults), approximately 46% of faults are predicted to have a 1 in 3 chance of being 604 unstable (i.e., $T_s > 0.3$, shown in red), and 54% of faults are predicted to have a 1 in 10 chance of being 605 unstable (shown in amber).



Figure 16. Output from the Monte Carlo modelling of slip tendency in UK coalfields. For slip tendency, more stable faults skew towards the left (low T_s), less stable faults skew to the right (high T_s). **a**. CDFs of predicted slip tendency for each mapped fault in South Wales. **b**. CDFs of predicted slip tendency for each mapped fault in Greater Manchester. Colour coding of CDFs – red: >33% chance of exceeding threshold friction (μ =0.3, vertical red line), amber: >1% and <33% chance, green: < 1% chance. Range of Byerlee friction shown by pink shading.

The results from the RSM/MC modelling shown in the CDFs are replicated in map view in Figures 17 and 18. Each fault segment is colour coded using the same heuristic applied in the CDF: red faults have a conditional probability of at least 33% of their slip tendency exceeding the chosen threshold value of fault rock friction (μ =0.3), amber (orange) faults have a 1-33% chance, and green faults have a less than 1% chance of being unstable.

618 For South Wales, the general pattern of the predictions is consistent with the recorded focal mechanisms (Figure 17a). The most likely fault segments to slip (coloured red) are those oriented either NNW/SSE or N/S, 619 620 corresponding with one of the nodal planes in each of the focal mechanisms. Faults trending ENE/WSW, such 621 as the Neath Disturbance, are predicted to have low probability of slip in the modelled stress regime (green). Note that the Swansea Valley Disturbance trends ENE/WSW as a fault zone, but the constituent fault 622 segments are variously oriented including elements that trend NE/SW, and these are marked in red (high 623 624 probability of slip). Blenkinsop et al. (1986) noted that this fault zone may in fact have a shallow dip at depth, 625 which is not covered by the dip distribution used in our modelling, so further work is required here. The 626 location with the most recorded events lies to the SE of Merthyr Tydfil, and this corresponds to an area with 627 many mapped faults trending NW/SE marked with a high probability of slip, and consistent with two of the 628 focal mechanisms.



Figure 17. Output from the Monte Carlo modelling of slip tendency in South Wales coalfield. **a**. Colour-coded fault map showing conditional probability of slip for each mapped fault. This map shows the unweighted values, as shown on the CDFs in Figure 14a. **b**. Colour-coded fault map showing conditional *weighted* probability of slip for each mapped fault. The weighted probability is calculated by multiplying the probability from the CDF in Figure 14a by the normalised fault smoothness, ranging from 1.0 for a perfectly straight (i.e., smooth) fault, and tending to 0.0 for a rough fault. Colour coding of CDFs – red: >33% chance of exceeding threshold friction (μ =0.3), amber: >1% and <33% chance, green: < 1% chance.

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For Greater Manchester (Figure 18a), the simulation suggests that many faults are likely to slip in the modelled stress regime, even though the recorded seismicity is generally sparse. The exception is the area of the 2002-2003 swarm near Manchester city centre. Here the recorded events coincide with mapped surface faults trending WNW/ESE and predicted as likely to slip (red).



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Figure 18. Output from the Monte Carlo modelling of slip tendency in Greater Manchester coalfield. **a**. Colour-coded fault map showing conditional probability of slip for each mapped fault. This map shows the unweighted values, as shown on the CDFs in Figure 14b. **b**. Colour-coded fault map showing conditional *weighted* probability of slip for each mapped fault. The weighted probability is calculated by multiplying the probability from the CDF in Figure 14b by the normalised fault smoothness, ranging from 1.0 for a perfectly straight (i.e., smooth) fault, and tending to 0.0 for a rough fault. Colour coding of CDFs – red: >33% chance of exceeding threshold friction (μ =0.3), amber: >1% and <33% chance, green: < 1% chance.

654

655 Discussion

656 Stress, pressure, and temperature

The simulations described in this paper all critically depend on our knowledge of the *in situ* stress tensor. We can constrain some of the components of this tensor better than others. The vertical stress (σ_v) is usually the best constrained, a reflection of its derivation from the borehole density logs sampled at sub-metre resolution. Our estimates of the horizontal stresses, σ_{Hmax} and σ_{hmin} , remain poorly constrained. Even in cases 661 with relatively good data, e.g., from borehole leak-off tests (LOTs) and formation integrity tests (FITs), the 662 "data density" for these stress components is generally sparse (compared to σ_V), and we are stuck with 663 significant uncertainties. And these uncertainties matter, as shown by this study and previous work (e.g., 664 Chiaramonte et al., 2008; Walsh & Zoback, 2016). The fundamental dependence of shear failure on 665 differential stress inherent in the Mohr-Coulomb failure criterion is reflected in the high ranking of stress 666 tensor components in the tornado plots shown in this study. Also, larger uncertainties in stress components mean that the Andersonian regime may flip from the default "average" assumption to another orientation: 667 668 e.g., an apparently strike-slip regime may in fact include a significant proportion of normal fault possibilities 669 (>20% in the case of the Porthtowan Fault Zone shown here). One way to improve our knowledge of the 670 stress tensor, and especially the azimuth of σ_{Hmax} would be to exploit richer catalogues of seismicity to 671 produce more focal mechanisms for natural or induced events. Most countries would benefit from better -672 i.e., more widespread and higher resolution – continuous seismic monitoring. While this may be expensive 673 with top of the range broadband equipment, citizen science devices, such as the Raspberry Shake, offer a 674 low cost and viable alternative (Cochran, 2018; Anthony et al., 2019; Hicks et al., 2021; Holmgren & Werner, 675 2021). Our study shows how Raspberry Shake data are effective for computing focal mechanisms. Analysis 676 of more events would allow stress inversions to be performed on the data measured by these devices, 677 especially when they are combined in *ad hoc* arrays to improve signal to noise ratios.

Pore fluid pressures at depth are also poorly known, even for a country like the UK with a long tradition of geological (and geophysical) science and rich history of mining and drilling into the crust. Most importantly, our knowledge of measured *in situ* pore fluid pressures in and around fault zones is generally poor. Theoretical predictions and model simulations abound, but direct measurements of this key parameter are almost non-existent. We need to know the actual limits of pore fluid pressures in fault zones, and their likely spatial and temporal variation over a fault plane throughout the seismic cycle.

The work described in this paper has ignored the effects of temperature. However, thermoelastic stress may be more important than poroelastic stress by a factor of 10 (Jacquey et al., 2015). In short, colder injected water may increase the chance of slip on a given fault. In the UK, our knowledge of the subsurface temperature field is increasing (Beamish & Busby, 2016; Farr et al., 2021), but we need more data, and again, especially from faulted rocks.

689 Faults

690 An implicit assumption in all of the modelling performed in this paper (and many others) is that we know 691 something about the fault which may slip: i.e., we can only quantify risk on known faults. There will, in 692 general, be many more unmapped faults in the subsurface, and these may be the ones most likely to slip due 693 to a change in loading (of either in situ stress or fluid pressure). This is apparent in the maps for the coalfields 694 shown in this paper in terms of the relative lack of correspondence between the surface mapped fault traces and the locations of recorded earthquakes. Some of this "mismatch" could be explained by the dip of the 695 696 faults measured at the surface, but not all. Moreover, there are areas of apparently intense surface faulting 697 and no recorded seismicity, and vice versa (recorded seismicity but no mapped surface faults). Some advance 698 could be made to address this problem with the recognition that each recorded seismic event documents a 699 fault plane, assuming that a double couple focal mechanism implies fault slip rather than dilation from dyke 700 emplacement or other mechanisms. And therefore the 3D position of each focal mechanism points to at least 701 part of a subsurface fault. The challenge then lies in mapping these seismic event fault planes into a viable 702 fault network. Better data (i.e., higher spatial resolution and extending to smaller event magnitudes) from 703 more dense arrays of seismometers would help with this task, as for the refinement of stress estimates noted 704 above.

705 Rock properties

The importance of good data on rock properties has been emphasised above, in the Worked Example for fracture susceptibility and in the case study for the Porthtowan Fault Zone. In general, we need more and better data on coefficients of friction and cohesive strength, especially for the target formations of decarbonisation operations. Moreover, we need data for the intact *and* faulted rocks. We also need better constrained correlations among rock properties. A widely used method in oil and gas is to derive estimates 711 of friction coefficient and UCS from wireline log datasets measuring porosity, slowness (velocity) or elasticity 712 e.g., Chang et al., 2006. However, as noted by these authors, the correlations are strictly valid only for the 713 specific formations tested in the laboratory, and even then, the uncertainties remain large. A further issue is 714 the tendency to average wireline log derived estimates over a depth interval, when for most sections of crust 715 this is the direction in which rock properties are expected to vary most rapidly. The Porthtowan Fault Zone 716 example above highlighted another issue: the relative impact of cohesion and friction on the predicted 717 stability depends on the magnitude of the cohesion in relation to the shear stress on the fault. For low 718 cohesion values, the constraints on friction become much more important. We need systematic 719 investigations of frictional behaviour at low cohesive strength. We need detailed systematic correlations 720 among rock properties, especially for faulted crystalline basement rocks.

Collecting more laboratory data is no panacea, evidenced by the well-aired concerns over how we up-scale rock properties and behaviours from mm- and cm-sized samples to whole fault zones. But calibrations and correlations from careful, systematic laboratory data remain the cornerstone of estimating the key *in situ* values. An interesting new focus would be to explore the nature of the skewness in mechanical property datasets: why should friction coefficients skew low, and cohesive strength skew high?

The utility of the Mohr-Coulomb criterion used in this paper is largely down to its mathematical simplicity, i.e., linearity and only two parameters (friction and cohesion). Other criteria are perfectly viable and could easily be added to the pfs Python code, but some other failure criteria lack a clear mapping between their parameters and the mechanics of sliding on rock surfaces.

730 Applicability of T_s, T_d and S_f for quantifying risk

731 A valid question is to ask whether any of these widely used measures of fault stability are, in fact, useful in 732 practical terms at the scale of faults on maps. All three measures focus on the simplified mechanics of slip on 733 a specific fault plane, with a fixed orientation and with specific rock properties. But seismic hazard is not 734 isolated at the level of single fault planes. Faults occur in patterns or networks, more or less linked together. 735 Geometrical factors may be more important than the specifics of either the in situ stress or the rock 736 properties, at the scale of observation. The observational record shows that bigger fault zones are the sites 737 of bigger earthquakes, and they are also the locus of most displacement in a given network. Conversely, 738 smaller faults host smaller seismic events, and accrue less overall displacement (Walsh et al., 2001). To begin 739 to address this issue, we can weight the conditional probabilities of slip for a specific fault segment by a 740 dimensionless normalised factor derived from the total length of the fault: e.g., $w_{size} = I_s / I_t$ where I_s is fault 741 segment length and I_t is fault trace length. An alternative, but related idea, is that of the relationship between 742 fault smoothness (or inversely, roughness) and fault maturity, and therefore seismic hazard (Wesnousky et 743 al., 1988). The most seismically active faults are not only, or necessarily, the largest ones in their network, 744 but tend to be the smoothest or most connected, reflecting the coalescence of fault segments through time 745 and the removal of asperities through repeated slip events (Stirling et al., 1996). Therefore, we can weight 746 the conditional probabilities of slip by a dimensionless factor of smoothness: $w_{smooth} = I_{straight} / sum(I_s)$, where 747 Istraight is the straight line length between fault end points, which is 1.0 for a perfectly smooth fault with all 748 segments parallel and connected, and tends to 0.0 for rough, complex fault traces. Examples of the effect of 749 these smoothness weightings applied to the conditional probabilities are shown in Figures 17b and 18b for 750 the UK coalfield faults. The net effect is to reduce the number of most risky faults (shown in red) by about 751 half. These approaches are the subject of further work and testing.

752

753 Summary

In this paper, we have described and explained the Response Surface Methodology and shown how it can be combined with a Monte Carlo approach to generate probabilistic estimates of fault stability using published measures of slip tendency, dilation tendency and fracture susceptibility. Simulations show that a quadratic response surface always generates a better fit to the input variables in comparison to a linear surface, at the cost of larger matrices (more computer memory) and longer run times. Worked examples to calculate T_s and S_f with synthetic input distributions show how the quadratic response surfaces vary for each input parameter. For slip and dilation tendency, the primary dependence is (as expected) on the maximum differential stress, and therefore the maximum and minimum principal stresses of the *in situ* stress tensor, with a lesser dependence on the fault orientation. For fracture susceptibility, the situation is more complex: if cohesion is relatively high, S_f is mainly dependent on the *in situ* stresses and cohesion. But if cohesion is low – quite likely in fault zones – then the dependence of S_f on friction is much more significant. This is a key finding: the relative sensitivity of the input variables on the response surface varies with the absolute value of the variables.

767 Sensitivity tests were used to assess how the shapes of different input distributions affect the predictions of 768 fault stability. Varying the spread of symmetric (normal, Gaussian) distributions of input variables has a 769 significant effect on the predictions, and this mirrors the reality of uncertainties in, for example, the principal 770 stresses in a standard geomechanical analysis. As noted above, the vertical stress is often well constrained 771 and has a lower relative standard deviation (say, 5% of the mean) than either the maximum or minimum 772 horizontal stresses (typically 15-20% of their mean value). The shape and spread of skewed (asymmetric) 773 distributions of rock properties (friction and cohesion) is also important. The direction of skewness is 774 described by the sign of the parameter α for the skewed normal distributions used in this paper to model 775 variations in rock properties. Friction is modelled with a negative skewness towards lower values, whereas 776 cohesion is modelled with positive skewness towards higher values, but systematic laboratory data are 777 needed to verify these assumptions. This will require a statistically significant number of repeat tests for each 778 property on quasi-identical samples of the same rock.

779 Case studies of three different locations demonstrated how a probabilistic approach can provide a useful 780 assessment of fault stability, including which of the input variables are the most important for a given 781 combination of *in situ* stress, fault plane orientation and rock properties. This then enables greater focus on 782 improving the estimates of the key variables, and the relationships between them. For the Porthtowan Fault 783 Zone in Cornwall, the modelling in this paper shows that we need more data for, and a better understanding 784 of the relationship between, coefficients of friction and cohesive strength, especially at low values of friction 785 (i.e., less than the Byerlee range of 0.6-0.85) to be expected in fault zones. For the coalfields in South Wales 786 and Greater Manchester, model outputs show how predictions of fault stability can be weighted by a simple 787 index of fault smoothness to begin to allow for the effects of geometrical weakening within the fault system 788 as whole, rather than focusing on each individual fault plane taken in isolation.

789 It's obvious that uncertainty in the input parameters must translate into uncertainty in the output 790 predictions. By combining a Response Surface Methodology with a Monte Carlo approach to the 791 quantification of fault stability, we can explore, understand, and quantify how differing degrees of 792 uncertainty among the input parameters feed through to uncertainty in the predicted stability measure. 793 Response surfaces and tornado plots can help to identify which parameters are the most important in a 794 particular analysis. Given our current state of knowledge of stress, fault orientations and fault rock 795 properties, probabilistic estimates and iterative modelling are useful approaches to begin to de-risk the 796 energy transition. Free, open source software to perform these analyses, such as the Python package pfs, 797 can help to encourage their wider adoption and further refinement ("given enough eyeballs, all bugs are 798 shallow"; Raymond, 2001). The deployment of abundant and relatively low-cost citizen science seismometers 799 (e.g., Raspberry Shakes) could synergise two critical issues: the wider involvement of the public into open science debates about risk and the simultaneous collection of better data to constrain the local stress field. 800 801 The energy transition and decarbonisation are urgent and essential tasks: we will only be successful if we 802 manage to balance public perceptions of risk with the technical challenges inherent to the exploitation of 803 faulted rock.

804

805 Appendix A – Dilation tendency plots

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For completeness, we include the analysis of dilation tendency (T_d) for the same synthetic input dataset used 807 to calculate slip tendency (T_s) – i.e., input variable distributions taken from Table 2.



808

809 Figure A1. Histograms of input variables used to calculate dilation tendency T_d for the synthetic distributions 810 shown in Table 2.



Figure A2. Residual plots for linear and quadratic response surfaces for dilation tendency using synthetic 811

data. The quadratic fit has a higher value of the adjusted R² parameter and is therefore deemed better in this 812 813 case.



Figure A3. Output from Monte Carlo simulation (N_{MC} =5,000) of dilation tendency calculated using a quadratic response surface from synthetic input data. **a**. Histogram of calculated dilation tendency values, in this case showing a quasi-normal distribution with a mode of ~0.75. **b**. Cumulative distribution function (CDF) of calculated dilation tendency values, showing the range in values from ~0.5 to ~0.9.

819

820 Code availability

- 821 <u>https://github.com/DaveHealy-github/pfs</u>
- 822
- 823 Data availability
- 824

825 Author contribution

- B26 DH 80%, SH 20%. DH originated the study, wrote the code, ran the models. SH contributed seismology
 data and expertise, and contributed to the writing of the text.
- 828

829 Competing interests

- 830 The authors declare that they have no conflicts of interest.
- 831

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