The Bayesian Earthquake Analysis Tool

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10 Abstract

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The Bayesian Earthquake Analysis Tool (BEAT) is an open-source python software to conduct source-parameter estimation studies for crustal deformation events, such as earthquakes and magma intrusions, by employing a Bayesian framework with a flexible problem definition. The software features functionality to calculate Green's functions for a homogeneous or a layered elastic half-space. Furthermore, algorithm(s) that explore the solution space may be selected from a suite of implemented samplers. If desired, BEAT's modular architecture allows for easy implementation of additional features, for example, alternative sampling algorithms. We demonstrate the functionality and performance of the package using five earthquake source estimation examples: a full moment-tensor estimation; a double-couple moment-tensor estimation; an estimation for a rectangular finite source; a static finite fault estimation with variable slip; and a full kinematic finite fault estimation with variable hypocenter location, rupture velocity and rupture duration. This software integrates many aspects of source studies and provides an extensive framework for joint use of geodetic and seismic data for non-linear sourceand noise-covariance estimation within layered elastic half-spaces. Furthermore, the software also provides an open platform for further methodological development and for reproducible source studies in the geophysical community.

27 1 Introduction

Crustal deformation processes, such as earthquakes, volcanic intrusions or due to human activities, 28 can have severe socio-economic impacts. For appropriate hazard assessment of these phenomena, 29 better understanding of the physical processes causing such deformation is required. An important step towards this goal is to carefully examine the geophysical observables caused by e.g. an 31 earthquake rupture, and then use these data to infer the spatial and temporal evolution of the 32 earthquake. The static surface deformation caused by such events can be measured by geodetic 33 techniques such as global navigation satellite systems (GNSS, e.g. GPS, Galileo and Glonass) and 34 Interferometric Synthetic Aperture Radar (InSAR) [e.g. Jónsson et al., 2002; Sudhaus and 2002; Sudha 35 son, 2009; Bathke et al., 2013. Rapid ground-surface displacements caused by a seismic wavefield, 36 on the other hand, can be measured with seismometers and in some cases GNSS. Both types of 37 38 measurements can be employed to study the characteristics of the deformation source by investi-

gating the inverse problem that relates source parameters to the observed data [e.g. Kikuchi and 39 40 Kanamori, 1982; Yagi and Fukahata, 2011]. Depending on the process being studied, the source can be parameterized in various ways. For 41 example, to explain displacements caused by a magma intrusion in the crust, an isotropic moment 42 tensor (MT) can sometimes be a reasonable approximation to model the observations [e.g. Bathke 43 et al., 2011; Biggs et al., 2014]. For earthquakes, a full or deviatoric MT [Jost and Herrmann, 44 1989; Tape and Tape, 2012; Sokos et al., 2012; Stähler and Sigloch, 2014; Tape and Tape, 2015] 45 in combination with a single source-time function may be sufficient to explain seismological obser-46 vations when the event is not large or is recorded at larger distances. However, the point-source 47 assumption of the MT is generally not valid for earthquake ruptures. Therefore, finite sources 48 with a spatial extent approximating earthquake fault planes have been applied. These include 49 simple rectangular sources [Haskell, 1964; Okada, 1985] and more complex finite-fault sources with 50 hundreds of source parameters [e.g. Olsen and Apsel, 1982; Hartzell and Heaton, 1983; Ji et al., 51 2002]. The variety of finite fault representations that have been used is large, even for the same 52 53 earthquake, as illustrated in the SRCMOD database [Mai and Thingbaijam, 2014]. For meaningful interpretation of estimation results, parameter uncertainties should be quanti-54 55 fied. These uncertainties are mostly caused by measurement errors and theory errors [Tarantola and Valette, 1982. The measurement error is partly due to data being contaminated by random 56 noise during measurement. This noise at seismic stations can be reduced, for example, by em-57 58 ploying better instruments and recording in low-noise environments. The most important error components in InSAR data are of atmospheric origin and may be reduced, for example, through 59 60 using additional independent data or through advanced processing strategies [Bekaert et al., 2015]. 61 Theory errors arise from assumptions in the mathematical formulation relating the model param-62 eters to the observed data. For example, layered models that simplify the velocity structure of the Earth are used in the computation of Green's functions [e.g. Yagi and Fukahata, 2011; Minson 63 et al., 2013; Duputel et al., 2014. Also, the parametrization of the deformation source, like the 64 discretization of the earthquake fault plane into a fixed number of patches, introduces theory errors 65 66 [Dettmer et al., 2014]. Parametrizations involving the source location, geometry and source-time-function are nonlin-

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early related to the surface displacements caused by the source. Consequently, inferring the source 68 69 parameters and uncertainties from displacements requires non-linear evaluation methods, which have high computational costs [Dettmer et al., 2007]. Bayesian inference is increasingly being ap-70 plied to solve nonlinear estimation problems as it has the advantage of quantifying uncertainties 71 of parameters [Monelli and Mai, 2008; Razafindrakoto and Mai, 2014] and prior information can 72 be consistently integrated in the problem definition [Xu et al., 2015; Dutta et al., 2018]. 73 74 Only a few software packages are available for nonlinear Bayesian inference combining static and dynamic displacement data (Tab. 1). For example, MTFit (Moment Tensor Fit) samples the 75 parameters of a full moment tensor while fixing the centroid location [Pugh and White, 2018]. 76 The algorithm considers amplitude ratios and the polarity of seismic phases. Although it does not 77 support seismic waveforms, the software is useful for seismic events of low moment magnitudes 78 $(M_w \sim 3)$. BayesISOLA (Bayesian Isolated Asperities) supports seismic waveforms to sample the 79 parameters of a full moment tensor in a mixed linear-nonlinear setting [Vackář et al., 2017]. The 80 location and source time are sampled via grid search and the moment-tensor components are 81 82 determined with a linear least-squares inversion. GBIS (Geodetic Bayesian Inversion Software) provides a Bayesian framework for sources with simple geometrical shapes (prolate spheroid, penny-83 84 shaped crack, etc.) [Bagnardi and Hooper, 2018] that have analytic closed form solutions, assuming a homogeneous elastic half-space Earth structure. Due to these source parameterizations GBIS is 85 limited to static surface displacement data, but can be useful in volcano geodesy (Tab. 1). While 86 87 the advantages of using Bayesian inference in deformation source estimations are undeniable, a software package that is sufficiently general for a wide range of applications has been lacking. 88 89 In this work, we present the Bayesian Earthquake Analysis Tool (BEAT), a general suite of 90 programs for a wide range of linear and nonlinear deformation source studies (Tab. 1, 2). BEAT provides the first open-source implementation for finite-fault estimations with variable static and/or 91 92 kinematic slip parameters (including hypocenter location) using Bayesian inference. Our approach can include static and/or dynamic deformation data and the user can specify which seismic phases 93 to include in the estimation. In addition, BEAT uses Green's function databases [Heimann, 2011; 94 95 Heimann et al., 2019 to speed up the source parameter estimations, where the user can also customize the 1D subsurface Earth structure. Finally, the software supports several sampling 96

algorithms that can be chosen depending on the problem to solve and the available computer resources. In conclusion, BEAT presents a complete open-source software infrastructure that can be applied to a wide range of problems and can also be extended by the user to foster future development of new methods, and to support reproducible research [Mai et al., 2016a,b].

101 2 Bayesian inference

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To estimate model parameters of a selected deformation source from geodetic/seismic data we apply Bayesian inference. The posterior probability density of the model parameters $p(\mathbf{m}|\mathbf{d}_{obs})$ can be obtained following Bayes' theorem

$$p(\mathbf{m}|\mathbf{d}_{obs}) \propto p(\mathbf{m})p(\mathbf{d}_{obs}|\mathbf{m}),$$
 (1)

where **m** is a vector of the parameters to estimate, i.e., the source parameters and optional hierarchical parameters (often called hyper-parameters), and \mathbf{d}_{obs} are observed data, i.e., seismic
waveforms and/or geodetic surface displacements.

A priori information is expressed through $p(\mathbf{m})$ for **m**, and $p(\mathbf{d}_{obs}|\mathbf{m})$ is the probability distribution of residuals (consisting of measurement and theory errors) for a given set of **m**. For a given

set of observed data, $p(\mathbf{d}_{obs}|\mathbf{m})$ is interpreted as the likelihood function $L(\mathbf{m})$, which quantifies the probability that a particular set of model parameters gave rise to the data. The observed data

 \mathbf{d}_{obs} can be regarded as the real quantity \mathbf{d}_{real} in addition to measurement errors \mathbf{e}_{meas} ,

$$\mathbf{d}_{obs} = \mathbf{d}_{real} + \mathbf{e}_{meas}.\tag{2}$$

The forward model $\mathbf{d}(\mathbf{m})$ simulates displacements generated by the chosen deformation source $\mathbf{d}_{\text{source}}$ and includes theory errors \mathbf{e}_{th} [Tarantola and Valette, 1982],

$$\mathbf{d}(\mathbf{m}) = \mathbf{d}_{\text{source}} + \mathbf{e}_{\text{th}}.\tag{3}$$

The theory errors result from assumptions and simplifications in the mathematical formulation of the forward model, e.g., from assuming a simple subsurface model that differs from the true subsurface structure. Typically, measurement errors and theory errors are not exactly known independently and probability distributions are thus commonly assumed to represent these errors.

In this study, we are mostly investigating nonlinear problems for which no analytic solution exists. Therefore, we have to solve the problems numerically. We assume a multivariate Gaussian distribution with error scaling σ_k to estimate the scale of the unknown distribution of residuals as a hierarchical parameter for each dataset $\mathbf{d}_{obs,k}$ [Fukuda and Johnson, 2008] of K datasets. Thus the PPD becomes

$$p(\mathbf{m}, \sigma_1, \sigma_2, ..., \sigma_K | \mathbf{d}_{obs,1}, \mathbf{d}_{obs,2}, ..., \mathbf{d}_{obs,K}) \propto p(\mathbf{m}) \cdot \prod_{k=1}^K L(\mathbf{m}, \sigma_k),$$
 (4)

124 with

$$L(\mathbf{m}, \sigma_k) = \frac{1}{(2\pi\sigma_k^2)^{N_k/2} |\mathbf{C}_{x_k}|^{1/2}} \exp\left[-\frac{1}{2\sigma_k^2} \left(\mathbf{d}_{obs,k} - \mathbf{d}_k(\mathbf{m})\right)^T \mathbf{C}_{x_k}^{-1} \left(\mathbf{d}_{obs,k} - \mathbf{d}_k(\mathbf{m})\right)\right], \quad (5)$$

where $\mathbf{d}(\mathbf{m})$ are the N_k predicted static or transient displacements for dataset k. The covariance matrix \mathbf{C}_{x_k} describes the variances and covariances of residuals for each dataset. The inverses of the covariance matrices in combination with the hierarchical scaling parameters σ_k act as weights for the different datasets. While BEAT includes significant infrastructure for addressing the covariance estimation, the details on the inference process are described elsewhere [Dettmer et al., 2007; Yagi and Fukahata, 2011; Duputel et al., 2014; Hallo and Gallovic, 2016].

131 2.1 Earth structure and Green's Functions

Before computing data predictions $\mathbf{d}(\mathbf{m})$ for a set of source mode parameters \mathbf{m} , we need to 132 133 make assumptions about the elastic subsurface structure. We assume the structure is a layered elastic half-space described by the density, thickness, seismic wave velocity and attenuation of each 134 layer. Once the subsurface structure has been defined, a linear combination of 10 (8 for the far 135 field) elementary Green's Functions (GFs) is needed to compute time-series of displacements for a 136 general moment-tensor source [Heimann, 2011; Heimann et al., 2019]. 137 138 The GFs are numerically expensive to compute and it is thus advantageous to pre-compute a 139 database of GFs prior to the model parameter estimation. Here, the software library pyrocko-gf is employed to generate databases of GFs [Heimann et al., 2019, 2017], which is an approach that 140 141 allows customizing the subsurface layering below each recording location. For example, the shallow subsurface structure from the CRUST2.0 model [Bassin et al., 2000] could be included for each 142 station to complement a common global Earth structure below the crust [Kennett et al., 1995]. 143

Estimation of the MT centroid location is possible once the GFs have been pre-computed for an 144 145 appropriate source-receiver volume, which requires that the source region is discretized with a GF 146 grid. 147 The GF databases are setup such that different programs can use them. Currently, support is included for QSEIS [Wang, 1999], QSSP [Wang et al., 2017] and PSGRN/PSCMP [Wang et al., 148 2006]. QSEIS calculates seismograms based on a layered visco-elastic half-space model and should 149 be used if local or regional setups are of interest. QSSP calculates seismograms based on a layered, 150 self-gravitating Earth and should be used for teleseismic setups or if interaction of the crust and 151 atmosphere is important. PSGRN/PSCMP calculates synthetic stress, strain, displacement, tilt 152 and gravitational fields on a layered visco-elastic halfspace and should be used for static displace-153 ment data. 154 Therefore, this infrastructure allows computing geodetic static displacements (at any depth) and 155 seismic waveforms at any distance and depth range with desired frequency content. In addition, 156

the open-source approach of BEAT makes extensions through user contributions straightforward

159 2.2 Estimation of source location and geometry

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to include.

The first order parameters of a deformation source are source location (east, north, depth), source-160 time-function (time, duration), and source geometry. These are determined in a nonlinear estima-161 162 tion (Eq. 5) and the number of source parameters **m** depends on the choice of deformation source. 163 BEAT supports a variety of point sources: a full moment tensor, an isotropic moment tensor, 164 a double-couple moment tensor and a compensated linear vector dipole (CLVD) moment tensor 165 (Tab. 2). By superposition of moment tensors, the GF database infrastructure permits discretizing 166 finite sources of arbitrary geometry and temporal evolution. For example, the parameters of a rectangular source [Haskell, 1964; Heimann, 2011] with unknown rupture nucleation and rupture 167 velocity can be inferred (Tab. 2, Supplemental Fig. S1, available in the electronic supplement to 168 this article). BEAT also allows for multiple sources of the same type, each with a full and indepen-169 170 dent set of source model parameters, allowing for custom and complex model setups. With this flexible setup, complex source shapes, such as caldera ring faults [e.g. Bathke et al., 2015], faults 171

with variable strike and dip [e.g. Dutta et al., 2019] and curved dike intrusions [e.g. Chadwick et al., 2011] can be studied.

174 2.3 Estimation of the slip history on a finite fault

For a finite fault source, under the assumption that the source fault geometry is known, the aim is to 175 176 resolve the spatio-temporal slip pattern on sub-faults. These sources are commonly discretized more 177 finely than can be resolved by data (over-parameterization), which requires regularization to avoid unstable solutions due to the ill-posed inverse problem [Altman and Gondzio, 1999]. Regularization 178 is typically applied via smoothness constraints based on a trade-off between slip smoothness and 179 data fit [Jónsson et al., 2002]. In Bayesian inference, smoothing regularization can be achieved via a 180 Gaussian prior $p(\mathbf{s}|\alpha)$, which includes a covariance matrix with off-diagonal terms, whose Cholesky 181 decomposition is equivalent to a Laplacian finite difference operator L of size $M \times M$. The trade-182 off parameter α scales the degree of smoothing and can be assumed to be an unknown parameter 183 (i.e., a hierarchical scaling that is estimated based on data information). Including smoothing 184 185 regularization of slip values s on M discretized fault patches, the PPD becomes [Fukuda and Johnson, 2008 186

$$p(\mathbf{m}, \sigma_1, \sigma_2, ..., \sigma_K | \mathbf{d}_{obs,1}, \mathbf{d}_{obs,2}, ..., \mathbf{d}_{obs,K}) \propto p(\mathbf{m}) \cdot p(\mathbf{s} | \alpha) \cdot \prod_{k=1}^K p(\mathbf{d}_{obs,k} | \mathbf{m}, \sigma_k),$$
(6)

187 with

$$p(\mathbf{s}|\alpha) = \frac{|\mathbf{L}^T \mathbf{L}|^{1/2}}{(2\pi\alpha^2)^{M/2}} \exp\left[-\frac{1}{2\alpha^2} (\mathbf{L}\mathbf{s})^T (\mathbf{L}\mathbf{s})\right].$$
(7)

Note that the application of Bayesian methods by themselves does not remove the need for regu-188 larization; it stems from the choice of spatial discretization of the fault. As long as the model is 189 over-parametrized, regularization is needed. However, Bayesian model selection can be applied to 190 overcome the need for regularization and subjective discretization choices [Dettmer et al., 2014]. 191 For static geodetic data, the slip values on the fault patches are linearly related to the resulting 192 surface displacements and $\mathbf{d}(\mathbf{m})$ reduces to \mathbf{Gm} . Here, \mathbf{G} is the sensitivity kernel containing dis-193 placement GFs for a source with unit slip for each slip direction (slip-parallel and slip-perpendicular) 194 on each sub-fault [Aki and Richards, 2002]. With seismic waveform data, kinematic rupture pa-195 196 rameters can be estimated. These include hypocenter location and time, rupture velocity and the 197 rupture duration. If rupture velocities are treated as an unknown velocity field on the fault, the Eikonal equation can be solved in each forward operation to ensure causal rupture propagation [Minson et al., 2013]. This leads to nonlinearity and G consists of two additional fields, i.e., the rupture duration and rupture start time on each slip patch for each seismic station.

201 In BEAT, G is referred to as a library and can be assembled given the source geometry and 202 the desired sub-fault discretization. This process requires a GF database to be pre-computed (see Sec. 2.1). When working with these libraries, it is useful to pre-compute them to make the 203 204 numerical sampling of the posterior computationally tractable and more efficient. However, the 205 libraries can be large for kinematic cases, leading to memory limitations. To overcome these 206 limitations, we recommend to apply as much a priori information about the source parameters as possible when defining the problem. For example, the rupture velocity of an earthquake is likely to 207 208 be close to the shear wave velocity of the subsurface medium [e.g. Das, 2015]. Consequently, the prior on the rupture velocity on each patch can be adjusted accordingly, if rupture propagation 209 with super shear wave velocity is not expected. 210

211 3 Sampling algorithms

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212 The posterior probability density (PPD) is usually numerically estimated through sampling with Markov Chain Monte Carlo (MCMC) methods [Sambridge and Mosegaard, 2002] or sequential 213 Monte Carlo (SMC) methods [Moral et al., 2006]. A commonly-used algorithm in the family of 214 215 MCMC samplers is Metropolis-Hastings sampling (MHS) [Metropolis et al., 1953]. In MHS, the 216 solution space is explored by a random walk, where the direction and size (or length) of a step is 217 randomly proposed by drawing from a probability distribution [Hastings, 1970]. A new state in 218 the random walk is accepted or rejected probabilistically; if the new state has a higher or equal 219 posterior probability than the current state, the new state is always accepted. If the new state has 220 a lower posterior probability, the new state is sometimes accepted and sometimes rejected. This 221 algorithm, samples directly from the PPD and allows to estimate general distributions where no closed-form solutions are available. 222 223

However, nonlinear source estimations often result in complex, multi-modal solutions that require advanced sampling algorithms in order to fully sample the complex multidimensional PPD and to avoid misleading results. For BEAT, we implemented three advanced sampling algorithms:

Adaptive Metropolis-Hastings (AMH) [Roberts and Rosenthal, 2001], Sequential Monte Carlo 226 (SMC) [Jarzynski, 1997; Neal, 2001; Moral et al., 2006; Ching and Chen, 2007; Minson et al., 227 2013] and Parallel Tempering (PT) [Geyer, 1991; Jasra et al., 2007; Dettmer and Dosso, 2012]. In 228 229 the following paragraphs, we give a short description of each algorithm and refer the reader to the 230 original publications for details. 231 The Adaptive Metropolis-Hastings algorithm tunes the step size of the proposal distribution based on the acceptance rate of the last N samples. If the acceptance rate is low, smaller steps 232 are proposed and vice versa. This algorithm is useful when sampling problems with only a few 233 234 model parameters; for example when estimating an isotropic moment tensor from geodetic data to resolve the location and volume change of a point source underneath a volcano [Kumagai et al., 235 236 2014]. In higher-dimensional problems, particularly with seismic data, the AMH algorithm appears to 237 238 be insufficient. Here, the SMC algorithm performs better due to its ability to temper the likelihood, apply resampling, and to take advantage of parallel computing. In the SMC algorithm, samples 239 240 are obtained by simulating a sequence of intermediate distributions from the prior to the posterior. Each sample starts from the prior and follows a trajectory through the intermediate distributions 241 242 to the posterior, where it is independent from other samples. The transitioning between distributions is typically achieved by scaling from the prior to the posterior via an annealing parameter 243 that allows samples to initially move freely in the parameter space, but gradually becomes more 244 245 constrained by the data as the sample approaches the posterior. At various stages, resampling can be applied to refocus the large number of samples into regions of high likelihood. This process 246 247 also helps the algorithm to avoid local minima. While slowly decreasing the annealing parameter 248 for each trajectory, a sample transitions through the bridging distributions until the PPD is sampled. The annealing enables sampling of complex, multi-modal and highly peaked distributions 249 since data information is gradually introduced. However, the number of trajectories needs to be 250 sufficiently large with respect to the number of parameters [Minson et al., 2013]. We implemented 251 the SMC algorithm with python's multiprocessing library, and consequently, this implementation 252 253 cannot scale beyond a single node of a computer cluster.

For parallel computing architectures (e.g. computer clusters), we implemented the PT algo-

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rithm with the Message Passing Interface (MPI). This algorithm generates many MCMC chains 255 256 in parallel (one per CPU), which draw samples from a joint posterior that includes the target posterior as well as tempered posteriors where the likelihood function is raised to a power of less 257 than unity. The chains are typically split such that half of the chains sample the target posterior 258 259 while the other half sample the tempered distributions. In addition, PT includes exchange moves, where various chains communicate and exchange information by swapping parameter vectors m. 260 261 The tempered posteriors significantly help the algorithm to widely explore the parameter space and reduce the tendency of getting stuck in modes. 262

263 4 Seismic covariance-matrix structure

In BEAT, the covariance matrices C_x for the seismic waveforms are estimated during the sampling, 264 based on data information and assumptions on the noise structure. It is important to note that 265 the noise covariance matrix substantially influences the Bayesian estimation result [Dettmer et al., 266 267 2007; Duputel et al., 2012. This matrix is generally not known a priori and it therefore has to be considered as a part of the estimation problem. However, as the residuals include theory errors 268 269 (see Eqs. 2, 3), this task is not trivial. In BEAT, three different forms of the covariance matrix are currently available: variance, exponential(toeplitz), non-toeplitz. For the variance and 270 exponential forms, the data variance is estimated from the seismic data by analyzing the data 271 272 variability prior to the P-phase arrival. The non-toeplitz matrix on the other hand, is estimated with an iterative approach and is based on the residual waveforms for the maximum a-posterior 273 274 (MAP) model parameters [Dettmer et al., 2007]. The non-Toeplitz covariance matrix accounts for 275 both non-stationary and correlated noise. As it is based on the residuals, it includes the effects 276 of both measurement errors and theory errors, e.g. due to inaccurate velocity structure of the subsurface. 277

278 5 Software features

279 BEAT is written in the python programming language and provides a Bayesian sampling frame-280 work for deformation source estimation. The project website, program prerequisites, platform and

license information can be found in Section 8. Several parts of BEAT are based on the pyrocko 281 seismological toolbox [Heimann et al., 2017]. The programming structure is object-oriented and 282 designed around two main estimation problems, which are referred to as modes and illustrated in 283 Fig. 1. The first mode, geometry, addresses the nonlinear problem of estimating the geometry, 284 285 source-time-function, location and magnitude or slip of the deformation sources (Sec. 2.2). The second mode, ffi (finite fault inversion), is used to estimate the spatially-variable static-slip values 286 287 or kinematic rupture parameters (Sec. 2.3). While the modes can operate independently, we rec-288 ommend to apply a geometry estimation prior to an ffi estimation. For example, if a geometry 289 estimation for a magnitude Mw > 6.5 earthquake yields a fault plane striking between 130 and 140 degrees, this information can be used in the ffi mode to constrain the fault geometry. Otherwise, 290 a reference fault geometry must be specified from other information. 291 292 A problem-specific yaml-configuration file (e.g. config_geometry.yaml in Fig. 2) provides an 293 interface for the user to adjust the various parameters of the problem, including prior information, data processing, and sampling-algorithm tuning. Two datatypes are supported in BEAT: 294 295 seismic (waveforms) and geodetic (GNSS and InSAR static displacements). The data types are 296 implemented in terms of composites that can be combined in the problem setup (Fig. 1). The 297 problem and composites classes include the formulation of the posterior likelihood (eq. 5), which is then synthesized to the model (Fig. 1) object that can be used by any sampler to explore the 298 solution space of the PPD. For numerical efficiency, the model is implemented via the open-source 299 300 libraries theano and pymc3, which provide the option to translate python code to C code, making it computationally more efficient, or to CUDA C code to make use of graphical processing units 301 (GPUs). 302 303 When using the software, the directory structure of the working directory gradually grows (Fig. 2). For example, the mode specific directories, such as geometry, are created during the 304

306 6 Application Examples

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307 To demonstrate the capabilities of BEAT, we present five different source estimation examples.

course of the sampling and the figures directory after the results are plotted.

nated them with synthetic correlated noise. These synthetic data were then used to estimate the 309 310 components of a full MT. In the other four examples, we considered both geodetic and seismic data of the 2009 L'Aquila earthquake. First, we estimate the location and the parameters of a 311 double-couple point source. Then, we employed a rectangular source to estimate the fault ge-312 313 ometry of the rupture assuming uniform slip. With the MAP parameters from the rectangular fault solution we then estimate spatially variable static slip, while keeping the fault geometry 314 315 fixed. Finally, we estimated kinematic parameters of the rupture based on the results of the previous two steps. Here, hypocentral location, rupture velocity and rupture duration were treated 316 as unknowns. These scenarios are fully reproducible and available as step-by-step tutorials at 317 https://hvasbath.github.io/beat/examples/index.html. 318 319 The uncertainty-quantification capability of BEAT and its flexibility can result in significant computational costs. The overall computation time depends on the amount of data, the complexity 320

of the source parametrization, and the available computational resources. In the following, we will

provide approximate computation times for the five estimation examples.

323 6.1 Example 1: Full Moment Tensor

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324 Here, we used the geometry mode to estimate parameters of a Mw5.5 MT source from simulated seismic data at regional distances up to 1000 km (Supplemental Fig. S2, available in the electronic 325 326 supplement to this article). Simulated waveforms were computed using a double-couple MT source 327 with a sinusoidal source-time-function (on $[0,\pi]$) and the simulated waveforms (Figs. S3 & S4 available in the electronic supplement to this article) were contaminated with simulated, temporally 328 329 and spatially correlated noise. To obtain such correlated noise for each waveform, we summed 330 up 300 synthesized waveforms containing the signals of random, full moment tensor sources in the 331 epicentral region $(\pm 3 \,\mathrm{km})$ with magnitudes between 3.0 and 4.7 and including five larger magnitude 332 sources between 4.5 and 5.0 with random source time variations between -20 and 5 seconds with 333 respect to the reference event. The corresponding signal-to-noise ratio varies between 1.2 and 3.3. 334 We applied SMC sampling with a MTsource parametrization to sample the parameters of a full 335 moment tensor, its centroid location and its source-time function.

To demonstrate the influence of different parametrizations for the data error covariance matrix

(Sec. 4), we compared results of sampling based on a diagonal covariance matrix (uncorrelated 337 338 noise, variance type in BEAT) and a non-Toeplitz, full covariance matrix, which accounts for time-dependent and non-stationary noise [Dettmer et al., 2007]. The comparison shows that the 339 double-couple mechanism was not retrieved in the estimation when neglecting noise correlations 340 341 (Fig. 3a,c), but was well recovered when using a non-toeplitz covariance matrix (Fig. 3b,d). With only data noise contamination in this synthetic test, the uncertainty of the solution is low for 342 343 the variance covariance-matrix case and the data are overfitted (Supplemental Fig. S5, S6 available in the electronic supplement to this article). However, this overfitting was reduced by using non-344 Toeplitz covariance matrices and the resulting parameter marginals are less biased (Supplemental 345 Fig. S7, S8, S9 available in the electronic supplement to this article), than when diagonal covariance 346 matrices were used. 347 For this example, we used 4 CPU cores on a standard mobile computer. We configured the 348 SMC sampler with 2,000 Markov chains over 300 steps over 40 stages. During the sampling, the 349

351 6.2 Example 2: Double-Couple Moment Tensor

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forward model was evaluated 24 million times, which took about 4 hours.

352 We considered data from the 2009 L'Aquila earthquake to estimate the double-couple momenttensor (DCSource) using the geometry mode of BEAT. We included P waveforms from 35 seismic 353 354 stations at teleseismic distances between 30 to 90 degrees (Supplemental Fig. S10, available in the 355 electronic supplement to this article). The seismic data were filtered with a Butterworth bandpass filter between 0.01 and 0.2 Hz. We applied a time window of -10 to +40 seconds around the 356 357 theoretical P-phase arrival time to calculate the posterior probability at each station. For the 358 seismic data we utilized the AK135 Earth velocity structure [Kennett et al., 1995] to compute a 359 GF database with QSSP [Wang et al., 2017]. To compare the results for two sampling algorithms on the PPD, we used PT and SMC sampling with the same setup. 360 361 For both sampling algorithms (PT and SMC), the mode and MAP of the marginals are similar 362 (Fig. 4). The estimated uncertainties in the source parameters are larger for PT compared to 363 SMC. Fuzzy waveform misfits (Supplemental Figs. S11, S12 available in the electronic supplement to this article) are comparable and uncertainties obtained from the SMC algorithm might be un-364

derestimated. These differences highlight that there is neither an ultimate measure nor a guarantee for convergence of sampling algorithms and the user must carefully evaluate posterior marginals estimated by the samplers [Mosegaard, 2012].

We configured the PT sampler with 20 chains and we randomly applied swaps every 10 to 369 30 steps. After each swap, we stored the sample of each Markov Chain that was sampled from the target PPD until 400k samples had been collected, which resulted in ~60 million forward evaluations and required ~5 hours of runtime. The SMC sampler was run with 5,000 Markov

Chains and 400 steps that resulted in 31 stages where the forward model has been evaluated \sim 62

374 6.3 Example 3: Rectangular Source Fault estimation

million times and required ~ 6 hours of runtime.

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Here, we used the seismic data from Example 2, and complement them with geodetic data to 375 estimate the fault dimensions and geometry for the L'Aquila earthquake using the geometry mode 376 of BEAT. The geodetic data were comprised of two InSAR surface displacement maps, derived 377 378 from Envisat satellite images acquired before and after the earthquake from both ascending and descending acquisition geometries (Supplemental Tab. S1, available in the electronic supplement 379 380 to this article). We applied the kite software [Isken et al., 2017] to spatially downsample the interferograms and to estimate the full data error variance-covariance matrix [Sudhaus and Jónsson, 381 382 2009; Jolivet et al., 2012. The AK135 Earth velocity structure [Kennett et al., 1995] was applied 383 to compute a GF database for the geodetic data with PSGRN/PSCMP [Wang et al., 2006]. The frequency band for the seismic data is broad compared to the previous example with 0.001 Hz 384 385 to 0.1 Hz, because the rectangular source with the rupture propagating across the fault produces 386 broad spectra. 387 We applied the SMC algorithm, a rectangular source parametrization and a non-Toeplitz seismic 388 covariance matrix to estimate the location, orientation, extent and slip of the L'Aquila source fault 389 (Supplemental Fig. S1, available in the electronic supplement to this article). In addition, we 390 estimated the rupture nucleation point assuming a constant rupture velocity of $3.5\,\mathrm{km/s}$ as well as 391 a source start time and duration of a half-sinusoidal source-time function. Finally, a hierarchical scaling was estimated (Eq. 4) for the interferograms and seismic data, as well as a bilinear ramp 392

function to account for possible inaccuracies in the satellite orbit information.

394 The results show that the strongest parameter trade-offs are between the extent of the fault (width and length), fault slip and the depth of the upper edge of the fault (Fig. 5). The horizontal 395 location of the rupture nucleation point is well constrained and located near the western edge of 396 397 the fault (nucleation x: -1 at left edge and 1 at right edge), while its downdip location is more uncertain, located somewhere near the bottom edge of the fault (nucleation y: -1 at the top edge 398 399 and 1 at bottom edge). The MAP model can explain the static surface displacement data well 400 (Supplemental Fig. S13, available in the electronic supplement to this article) and the simulated 401 waveforms also show a good agreement with the observations, considering that only uniform fault slip was included in this model estimation (Supplemental Fig. S14, available in the electronic 402 supplement to this article). 403 In this example, we again used 4 mobile CPU cores to sample 1,000 Markov chains with 100 404 steps each and through 22 stages of the SMC sampler. This resulted in ~ 2.2 million forward 405

407 6.4 Example 4: Static slip-distribution estimation with Laplacian smooth-

evaluations and over 11 hours of computation time.

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409 In this example we consider a finite fault parametrization for the L'Aquila earthquake and the ffi mode of BEAT using the static InSAR data. We employed the previously determined parameters 410 411 from the rectangular source estimation (Sec. 6.3) to fix the source fault location and geometry as well as the orbital ramps for the InSAR scenes. We extended the previously obtained MAP fault 412 dimensions in length by a factor of 1.6 and in width by a factor of 1.4. Then, we discretized the fault 413 into 2×2 km patches resulting in 121 patches (11 × 11). For each of these patches, we computed GFs 414 slip-parallel and perpendicular to fault rake. While assuming smooth slip on neighboring patches 415 416 (Laplacian smoothing; Eq. 7), we applied the SMC algorithm to solve for the two slip parameters on each patch as well as estimating the smoothing parameter and hierarchical scaling for each 417 interferogram (Eq. 4). The number of parameters estimated in this example is 245, i.e., two slip parameters for each patch, one smoothing parameter and two hierarchical scaling parameters. To 419 initialize each Markov Chain at a reasonable starting point of the high-dimensional search space, 420

we drew a random smoothing weight α from its prior (uniform) distribution. With these smoothing values we inverted for the rake-parallel slip distribution via regularized non-negative least-squares [Fukuda and Johnson, 2008]. The resulting slip vectors in the slip-parallel direction and zero slip in the slip-perpendicular direction were set as the starting points for the MCs in the first stage of the SMC algorithm.

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The fault slip distribution results (Fig. 6) show a maximum slip of ~0.7 m and significant slip confined between 2 and 18 km. The slip uncertainties increase with depth as the ability of static surface displacements to resolve fault slip decreases with depth. This solution does not consider uncertainties in location and geometry as found in Example 3 (Fig. 5). These would enlarge the slip vector error ellipses [Sudhaus and Jónsson, 2009, 2011]. The model prediction of this variable fault slip model fits the observed InSAR data better than the previous constant slip model (Supplemental Fig. S15, available in the electronic supplement to this article).

We carried out this model parameter estimation on 4 mobile CPU cores as before and included sampling of 3,000 Markov chains for 300 steps over 43 stages of the SMC sampler. During the sampling the forward model was evaluated 39 million times, which took about 3 hours.

The assumption of smooth slip between neighboring slip patches can sometimes be inappropriate [Minson et al., 2013; Duputel et al., 2014; Ragon et al., 2018]. Thus, BEAT also supports estimating distributed slip without a Laplacian smoothing prior, but instead the uncertainty in Earth structure is propagated [Duputel et al., 2014] (Supplemental Sec. 1, Figs. S16-S22, available in the electronic supplement to this article).

441 6.5 Example 5: Kinematic nonlinear slip estimation with Laplacian 442 smoothing

In this final example we extended the L'Aquila source estimation to include rupture kinematics and used both seismic waveforms and static InSAR data as observations. To increase the data information about the rupture details, we filtered the waveforms with an upper limit of 0.5 Hz and we extended time windows around P-wave arrivals to -10 s to 50 s. For the estimation, we applied the ffi mode of BEAT and used the posterior slip distribution result of example 4 as a slip prior to reduce the parameter space. The kinematic rupture parameters that we estimated include the

hypocenter time and location as well as the rupture velocity and duration on each fault patch. In 449 450 addition, we estimated smoothing parameter α and hierarchical residual scaling parameters. The total parameter count in this example is 491, i.e., four kinematic slip parameters for each of the 451 121 patches, three hypocenter parameters, one smoothing parameter, and three scaling parameters 452 453 for the two InSAR datasets and the seismic data. We applied the SMC sampler in the estimation, assuming a non-Toeplitz seismic covariance matrix, with Markov Chains initialized to the posterior 454 455 from the previous example, as we considered it as prior information. 456 The kinematic results show that the hypocenter location is well constrained, and that the rupture nucleated near the western edge of the fault at a depth between 10 and 12 km (Fig. 7 457 a). The rupture appears to have spread with near constant rupture velocity of $\sim 3 \,\mathrm{km/s}$ across 458 the fault. Compared to the static solution, the maximum slip is reduced to $\sim 0.6 \,\mathrm{m}$ and the slip 459 distribution is overall somewhat shallower (by $\sim 2 \text{ km}$), i.e., it is now mostly confined to depths less 460 than 16 km. Due to the addition of seismic data, rake and slip uncertainties on deep slip patches are 461 significantly reduced. Marginal distributions of selected patches (Supplemental Fig. S23, available 462 463 in the electronic supplement to this article) show that the kinematic slip parameters for patches far from the hypocenter (e.g. patch 15) are poorly resolved, with the 95% confidence bounds on the 464 465 rupture duration and rupture velocity, between 0.5 and 2.6 seconds and between 2.5 and 4.3 km/s, respectively. This is not be surprising as only teleseismic data were used in the estimation. Patches 466 with high slip values have shorter rupture durations (e.g. patch 51) with the 95% confidence bounds 467 468 between 0.1 and 2 seconds. The rupture velocities of patches close to the hypocenter (e.g. patch 67) are slightly better constrained (with the 95% confidence bounds between 2.45 and 3.8 km/s) than 469 470 patches further away. Note that this kinematic solution includes an estimation of the smoothing 471 weight α and the result is based on a range of α values rather than a single fixed smoothing value (Fig. 7 c). The moment rate function shows a source rupture duration of $\sim 9-10$ s with the 472 peak moment release occurring between 4s and 6s (Fig. 7b). The fit with the geodetic data is 473 comparable to Example 4 (Fig. 8), but the fit with the seismic waveforms (Fig. 9) appears to be 474 poorer than in Examples 2 and 3. The latter comparison, however, is unfair as the seismic data in 475 476 this example include significantly more details due to the increased upper cut-off frequency of the bandpass filter. 477

Several features from our results generally agree with previous studies. The rupture exhibits predominantly a single slip region at depths between 5 and 16 km. The hypocenter is located in the northwest and offset from the main slip region [Cirella et al., 2009; Zhang et al., 2012]. The moment rate function (Fig. 7) shows a small peak near 2 s. Finally, the rake angle indicates a slight rotation of the slip vector with increasing depth [Zhang et al., 2012].

In this example we employed 25 cores on a workstation to sample 10,000 Markov chains for 300 steps over 35 stages of the SMC sampler. This resulted in \sim 100 million forward model evaluations

486 7 Conclusions

and a runtime of ~ 85 hours.

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The Bayesian Earthquake Analysis Tool (BEAT) is a new software for source estimations and 487 uncertainty quantification in deformation source studies. It is open source and available under the 488 license GPL3.0 and can be downloaded at https://github.com/hvasbath/beat [Vasyura-Bathke 489 490 et al., 2019. BEAT provides an extensive open source framework to study earthquake sources with various parameterizations, including moment-tensor point sources, rectangular static and 491 492 kinematic sources, and static and kinematic finite fault sources. An important aspect of BEAT's contribution is the integration of multiple methods in a unified platform. In addition, we provide 493 the novel ability to consider joint inversion of geodetic and seismic data for sources in a stratified, 494 495 elastic half space with residual covariance estimation, while allowing fully non-linear treatment of all sources in a Bayesian framework. The intention behind providing such a unified framework to the 496 497 geophysics community is to make research more reproducible and to accelerate the development of 498 comprehensive tools for deformation source studies. The five examples presented here demonstrate 499 the main functionalities of the BEAT software and can be reproduced through step-by-step tutorials available on the project website: https://hvasbath.github.io/beat/examples/index.html. 500

8 Data and Ressources

The BEAT package runs under Linux and MacOS on python versions =< 3.5 and is available at https://github.com/hvasbath/beat [Vasyura-Bathke et al., 2019]. It is distributed under the

- 504 GNU General Public Licences, version 3.0 and depends on the following main python libraries
- 505 (and dependencies within): pyrocko [Heimann et al., 2017], pymc3 [Salvatier et al., 2015], Theano
- 506 [Theano Development Team, 2016] and MPI4py [Dalcin et al., 2011].
- The presented examples can be reproduced following the tutorials at: https://hvasbath.
- 508 github.io/beat/examples/index.html.
- 509 Seismic waveforms were originally downloaded from Incorporated Research Institutions for
- 510 Seismology (IRIS) https://ds.iris.edu. Envisat satellite radar data were provided by the European
- 511 Space Agency (ESA) https://earth.esa.int/web/guest/home.
- All of the figures have been produced by using matplotlib [Hunter, 2007] and can be generated
- 513 through the BEAT plot command. Some maps have been produced by using Cartopy [Met Office,
- 514 <u>2015</u>].
- 515 Supplemental Material for this article includes a pdf file further illustrating the examples.

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733 Figure 1: The BEAT modular program structure. The main problem objects determine, to-734 gether with their composites, the model that contains the rules to calculate the posterior probability. To date, BEAT contains two problem classes, the geometry problem (Sec. 2.2) and the 735 finite-fault estimation problem (Sec.: 2.3). These are being used by the sampler objects to explore 736 737 the solution space of their respective PPD. 738 739 Figure 2: An example of a directory tree for a BEAT project after all steps have been executed. The config_*.yaml files are the parameter files to configure and customize the sampling pro-740 cess. The results directory (created by command export) contains sampling results, estimated covariance matrices and synthetics. The hypers directory contains sampling results of the initial 742 743 hyper-parameter estimation. The linear_gfs directory contains the Green's functions for the finite-fault-inversion (created by command build_gfs). stage_* folders contain results of the dif-744 ferent sampling stages of the SMC sampler ("*" represents the integer number of the corresponding 745 stage) and stage_-1 contains the PPD of the model parameters of the corresponding final stage. 746 747 Figure 3: Results of Example 1: (a) and (b) Hudson plots from ensembles of 1000 moment-tensor 748 solutions (small black beachballs) for estimations using variance and non-Toeplitz covariance data-749 covariance matrices, respectively. The large red and grey beachballs show the MAP solutions and 750 the true moment tensor, respectively. (c) and (d) fuzzy beachballs based on ensembles of 1000 751 752 MT solutions drawn from the PPD of the two estimations using the variance and non-Toeplitz 753 data-covariance matrices, respectively. 754 755 Figure 4: Results of Example 2: Marginal posterior distributions for model parameters of a double-756 couple source estimated from real teleseismic data of the L'Aquila earthquake obtained from two different sampling algorithms, Sequential Monte Carlo (SMC, yellow) and Parallel Tempering (PT, 757 blue). The MAP values are marked by vertical colored lines. 758

760 Figure 5: Results of Example 3: 1D and 2D marginal posteriors of a rectangular source for the

761 L'Aquila earthquake. The red vertical lines in the histograms and the red dot in the 2d correlation

762 maps mark the MAP solution. In the correlation plots, blue colors are regions of high probability.

763 North and East shifts are relative to a given reference location.

764

765 Figure 6: Results of Example 4: a) Static slip distribution solution for the L'Aquila 2009 earth-

766 quake estimated using static InSAR surface displacements. The patch colors and the black arrows

767 show the MAP, whereas the black ellipses around the arrow tips show the two-sigma confidence

768 bounds.

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770 Figure 7: Results of Example 5: (a) Kinematic slip distribution for the L'Aquila 2009 earthquake

771 from the joint inference on teleseismic and InSAR static data. The patch colors and the black

arrows show the MAP, whereas the black ellipses around the arrow tips indicate the two-sigma

773 confidence boundaries, and the black star marks the hypocentral location. The black continuous

1774 lines show the MAP of the evolving rupture front, with the timing of each front in seconds anno-

775 tated on the respective isoline. The uncertainty of the rupture onset time is shown as the fuzzy

isolines with light grey indicating lower probability. (b) The ensemble of moment rate function

solutions, with dark and red colors indicating high probability moment rates. The continuous black

line shows the MAP moment rate function. (c) Marginal posterior distribution for the Laplacian

779 smoothing weight α , with the red vertical line marking the MAP solution.

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781 Figure 8: Results of Example 5: geodetic InSAR data fits for the L'Aquila earthquake from

782 descending (a) and ascending (b) acquisition geometry. (data panels) Geocoded unwrapped in-

783 terferograms in radar line-of-sight (LOS) with negative values indicating increasing LOS distance

due to subsidence. The displayed displacement values are derived from quadtree subsampling and

785 extrapolated to each pixel that belong to the same quadtree square. The look-vector and heading

of the satellite are shown by the two short and long arrows, respectively. (model panels) Synthetic

surface displacements in LOS derived from the MAP solution. The small grey rectangle shows

788 the location and orientation of the derived fault geometry from example 2, whereas the red rect-

angle shows the extended fault geometry that is used in examples 3 and 4. The solid black lines

790 mark the upper edge of the fault. (residual panels) Residual surface displacements, i.e., the dif-791 ference between the model and the data panels. Note the different color scale for the residual plots.

792

Figure 9: Results of Example 5: Waveform fits for the kinematic finite fault solution for P-793 wave arrivals for 16 of the 35 stations used. The filtered (0.001-0.5Hz) displacement waveform 794 data (dark grey solid line) and the filtered synthetic displacement waveforms (red solid line) are 795 shown together, with the brown shading indicating 100 random draws of the filtered synthetic 796 797 displacements from the PPD. The residual waveforms are shown below each waveform as filled red-line polygons. Each trace box is annotated with the station name and component, as well as 798 the distance and azimuth from the MAP solution of the center of the reference fault. The arrival 799 800 time and the duration of each window are shown in the lower left and right, respectively.

801 Tables

Table 1: Recent, open source software for Bayesian estimation of deformation sources.

NAME	UQ, Samplers ^a	SOURCE TYPES	SOURCE TIME	DATA TYPES	GF	References
			${ t FUNCTION}({ m STF})$		SUP-	
					$PORT^{b}$	
MTfit	Bayesian, MH^c , RJM -	single source, linear full MT f , DC g	no	wave polarity, wave amplitude	ou	[Pugh and
	CMC^d , MC^e			ratios		White, 2018]
GBIS	Bayesian, AMH^h	multiple sources, isotropic point,	no	static displacments (GNSS i , In- half-	half-	[Bagnardi
		spherical, rectangular, penny-		SAR^j	space	and Hooper,
		shaped crack, ellipsoid			only	2018]
Bayes	Bayesian, grid search,	single source, quasi-nonlinear full	no	seismogram waveforms	yes	[Vackář
ISOLA	LSQ^k	MT				et al., 2017]
BEAT	Bayesian, AMH, SMC^l ,	multiple sources, nonlinear full MT,	half-sinusoidal, tri-	seismogram waveforms, static	yes	this work
	PT^m	rectangular source, isotropic MT,	angular, boxcar	displacements (GNSS, InSAR)		
		CLVD^n , DC ; full kinematic/static				
		finite-fault				

 $[^]a\mathrm{UQ}\text{-}$ uncertainty quantification

 $[^]b \mathrm{GF} ext{-}$ Green's Function

cMH- Metropolis-Hastings

 $[^]d\mathrm{RJMCMC}$ - reversible jump markov chain monte carlo

 $[^]e\mathrm{MC}\text{-}$ Monte Carlo random sampling

fMT- moment tensor

 $[^]g\mathrm{DC}$ - double couple

 $[^]h\mathrm{AMH}\text{-}$ Adaptive Metropolis-Hastings

^{&#}x27;GNSS- global navigation satellite system

 $^{^{}j}\mathrm{InSAR}\text{-}$ interferometric synthetic aperture radar

 $[^]k\mathrm{LSQ}\text{-}$ least squares inversion

 $[^]l\mathrm{SMC}\text{-}$ sequential Monte Carlo

 $[^]m$ PT- parallel tempering

 $^{^{}n}\mathrm{CLVD}\text{-}$ compensated linear vector dipole

Table 2: Types of deformation sources and their source specific parameters that can be estimated in the geometry mode of BEAT.

DEFORMATION	Parameters m	References
Source		
Full moment tensor	$m_{nn}, m_{ee}, m_{dd}, m_{ne}, m_{nd}, m_{ed}, $ mo-	[Stähler and Sigloch, 2014]
(MT) I	ment magnitude	
Full moment tensor	u, v, κ , σ , h, moment magnitude	[Tape and Tape, 2015]
(MT) II		
Isotropic moment	moment magnitude or volume change	[Kumagai et al., 2014]
tensor		
Double couple	strike, dip, rake, moment magnitude	[Jost and Herrmann, 1989]
(DC)		
Compensated lin-	dip, azimuth (of largest dipole), mo-	[Jost and Herrmann, 1989]
ear vector dipole	ment magnitude	
(CLVD)		
Rectangular source	strike, dip, rake, length, width, slip, op-	[Haskell, 1964]
	tional: hypocentral location (x,y), rup-	
	ture velocity	

802 10 Figures

















