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Simulator-Based Bayesian Inference of Enhanced Geothermal Reservoir Properties

Kwabena Atobra¹ , Gregor Hillers^{1,2} , Vladimir Lyakhovsky³ , Eyal Shalev³ ,
Arto Klami⁴, and Ulpu Remes⁵

¹Institute of Seismology, University of Helsinki, Helsinki, Finland, ²Geothermal Energy and Reservoir Technology, Institute of Applied Geosciences, Karlsruhe Institute of Technology, Karlsruhe, Germany, ³Geological Survey of Israel, Jerusalem, Israel, ⁴Department of Computer Science, University of Helsinki, Helsinki, Finland, ⁵Department of Mathematics and Statistics, University of Helsinki, Helsinki, Finland

Key Points:

- Bayesian optimization for likelihood-free inference supports geothermal reservoir parameter estimation based on limited forward evaluations
- The HydroPED simulator uses viscoelastic damage rheology modeling to evaluate the seismo-hydraulic state of a geothermal system
- The potency target function encodes the spatial distribution of the energy release better than a simpler seismic event count approach

Correspondence to:

K. Atobra,
kwabena.atobra@helsinki.fi

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Author Contributions:

Conceptualization: Kwabena Atobra, Gregor Hillers, Arto Klami
Data curation: Kwabena Atobra
Formal analysis: Kwabena Atobra
Investigation: Kwabena Atobra
Methodology: Kwabena Atobra, Gregor Hillers, Vladimir Lyakhovsky, Eyal Shalev, Arto Klami, Ulpu Remes
Project administration: Gregor Hillers
Software: Vladimir Lyakhovsky, Eyal Shalev, Ulpu Remes
Supervision: Gregor Hillers, Vladimir Lyakhovsky, Eyal Shalev, Arto Klami
Validation: Vladimir Lyakhovsky, Eyal Shalev, Ulpu Remes

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Abstract Inversions of dynamic multi-scale multi-physics subsurface system properties rely on the effective sampling of high-dimensional parameter spaces and are thus notoriously difficult to perform. The associated models are defined by complex nonlinear relationships with potentially stochastic components, which lead to analytically intractable likelihoods that require challenging forward simulations of the system response. This paper presents the application of the Bayesian optimization for likelihood-free inference (BOLFI) algorithm to invert the properties of a geothermal reservoir. We use the viscoelastic damage rheology simulator HydroPED to model an enhanced geothermal system (EGS) with controlled reservoir properties. Our results demonstrate the effectiveness of combining BOLFI and the computationally expensive simulator HydroPED to estimate an informative posterior distribution from a comparatively small number of forward evaluations. In this pilot, we use BOLFI to invert for ambient principal stress values using synthetic target data. We parameterize the 2-km scale reservoir with ~16'000 elements and perform tests with 200 and 500 HydroPED forward simulations that each take a wall-clock time of 1.5 hr using an 8-core CPU node to simulate one day of a hydraulic stimulation. Using potency, which encodes the spatial distribution of energy release within the simulator reservoir as a target function for the inversion, yields better results compared to a simpler event count target function. The approach we use in this study can be extended to a wide range of seismic and hydraulic target observations to constrain ambient stress and local EGS model parameters.

Plain Language Summary This study explores a new way of estimating the parameters of geothermal reservoirs, such as stresses, using an inversion algorithm called Bayesian optimization for likelihood-free inference (BOLFI). BOLFI allows us to predict the approximate values of the principal stresses found in a simulated geothermal reservoir. We perform the simulation with a computer program called HydroPED, which takes stress values as inputs and generates a catalog of seismic events, amongst other outputs such as damage distribution, fluid pressure distribution, and rock pressure distribution. We analyze the catalogs produced to obtain the potency and number of events for each simulation done, and BOLFI uses that information to help choose the next stress values to simulate with. We obtain better results when we use the potency, a measure of how faults slip during seismic events, rather than using the event count.

1. Introduction

Inverse problems are common in geophysics for estimating subsurface properties from noisy and incomplete observations (Sambridge, 1999a). Robust inversion is critical for Enhanced Geothermal Systems (EGSs), where hydraulic stimulation modifies permeability and induces seismicity through coupled changes in stress, damage, fluid flow, and temperature (Li et al., 2021). Effective inversion methods are therefore needed to characterize evolving reservoir properties and support safe, economically viable operations.

Generally, inverse methods combine observations, a forward model, and a sampling or optimization strategy. They are often categorized as gradient-based or direct search approaches (Sambridge, 1999b). Gradient-based methods can be efficient for mildly nonlinear problems but may struggle with strong nonlinearity and are prone to getting stuck in a local minima (Sambridge, 1999b). Direct search methods avoid computing derivatives and can better handle nonlinear models. Examples include simulated annealing, genetic algorithms, and the neighborhood algorithm (Sambridge, 1999b). Simulated annealing uses a temperature-controlled sampling density function and has been applied in waveform and electromagnetic inversions (Shiba & Irikura, 2005; Tang

Visualization: Kwabena Atobra

Writing – original draft:

Kwabena Atobra

Writing – review & editing:

Kwabena Atobra, Gregor Hillers,
Vladimir Lyakhovsky, Eyal Shalev,
Arto Klami, Ulpu Remes

et al., 2024). The neighborhood algorithm approximates the misfit surface using Voronoi cells and is useful when the objective has multiple local minima (Coutand et al., 2014; Sambridge, 1999b; Steffen & Kaufmann, 2005; Wathelet, 2008). These direct-search approaches are flexible but can still be computationally expensive for high-dimensional, nonlinear, and stochastic forward models. This motivates machine-learning (ML) approaches that can accelerate repeated forward evaluations to speed up the inversion.

ML based inverse methods build data-driven surrogate or reduced-order models (ROMs), similar to the first step in the neighborhood algorithm. For example, Schleder et al. (2019) inverted atomic structures for materials design, and Willard et al. (2020) inverted 3D human-body structure from x-ray images. ML-based ROMs can accelerate inversion by acting as faster forward evaluators: they can replace a full-order model, emulate dimensionality-reduction mappings, or learn residuals between an existing ROM and observations (Agiza et al., 2012; Mohan & Gaitonde, 2018; Wan et al., 2018). Neural networks can also improve forward evaluations and calibrate sensitive parameters for subsequent simulations (Sharifi et al., 2019). Finally, ML can support likelihood-free, simulator-based Bayesian inference when the likelihood is intractable. A broad class of simulation-based inference (SBI) methods learns neural surrogates of the posterior, likelihood, or likelihood ratio, enabling fast amortized inference but typically requiring large numbers of simulator runs for training (Papamakarios, 2019). In this work we instead adopt BOLFI (Gutmann & Corander, 2016), which is designed for expensive simulators and small evaluation budgets. BOLFI uses active learning to build a Gaussian-process surrogate of the discrepancy and selects the next simulation points via an acquisition rule. Conceptually, this places BOLFI within likelihood-free Bayesian inference as a sequential, surrogate-assisted alternative to both rejection-style Approximate Bayesian Computation (ABC) and amortized neural SBI. Accordingly, the specific methodological contribution of this work is not a new SBI algorithm but the demonstration that BOLFI can be coupled to the quasi-stochastic seismo-hydromechanical forward model HydroPED to obtain informative stress posteriors under tight simulator budgets, and to quantify how summary-statistic choice controls posterior robustness.

An EGS is a multiscale, multiphysics reservoir that often requires coupled seismo-thermo-hydro-mechanical and potentially -chemical (STHMC) modeling. Simulators used to model EGS include equivalent-continuum models, discrete-fracture-network models, discrete-fracture models, and embedded-discrete-fracture models, which trade physical fidelity for computational efficiency (Boillat, 2003; Fadakar Alghalandis, 2017; Li et al., 2021; Pandey et al., 2017; Yao et al., 2018). Common THM/THMC platforms include TOUGH-FLAC/TOUGHREACT-FLAC3D, THAMES, MOTIF, FRACON, PANDAS, OpenGeoSys, Dumux, and COMSOL (Flemisch et al., 2011; Kolditz et al., 2012; Olin et al., 2008; Rutqvist, 2011, 2017; Xing et al., 2015). Rutqvist, Dobson, et al. (2013) used THM modeling at the Northwest Geysers (California) to predict stimulation extent and seismicity features. However induced seismicity is not universally represented, and many simulators (e.g., TOUGH-FLAC, Rockflow, and COMSOL) lack explicit coupling between damage-driven stress drops, earthquake mechanics, and pressure diffusion, and omit key damage mechanisms such as stress-reversal effects and dilatancy. Together with the inherent stochasticity of seismic observations, this limits conventional inversion methods that assume deterministic forward models or tractable likelihoods (Andrés et al., 2022; Rutqvist, Rinaldi, et al., 2013; Xing et al., 2015).

Traditional inversion often requires thousands to millions of forward evaluations for highly nonlinear dynamics and can break down for stochastic forward models, effectively restricting inference to fast and often linearizable simulators. We apply an ML-accelerated, likelihood-free workflow to ambient-stress inversion in an EGS using a quasi-stochastic forward simulator to generate a synthetic reservoir response. HydroPED provides the forward model, BOLFI provides likelihood-free sampling, and Markov Chain Monte Carlo (MCMC) is used to sample the posterior.

In this study, we explore the effectiveness of combining HydroPED and BOLFI to monitor reservoir properties. We focus on the inversion of the ambient in situ principal stresses as an example of an important reservoir property useful for many subsurface engineering projects. Generally, stress estimates can be obtained from geological indicators (Morris et al., 1996), hydraulic fracturing and minifrac experiments (Dahm et al., 2010; Zoback, 2010), borehole breakout observations (Zoback, 2010), overcoring and other configurations involving strain gauges (Zoback & Mary, 1992), and from properties of seismicity patterns (Schorlemmer et al., 2005) and individual earthquakes (Boyd et al., 2018; Martínez-Garzón et al., 2013; Vavryčuk, 2014). However, obtaining reliable estimates of the stress direction and magnitudes remains challenging, and extrapolations from regional

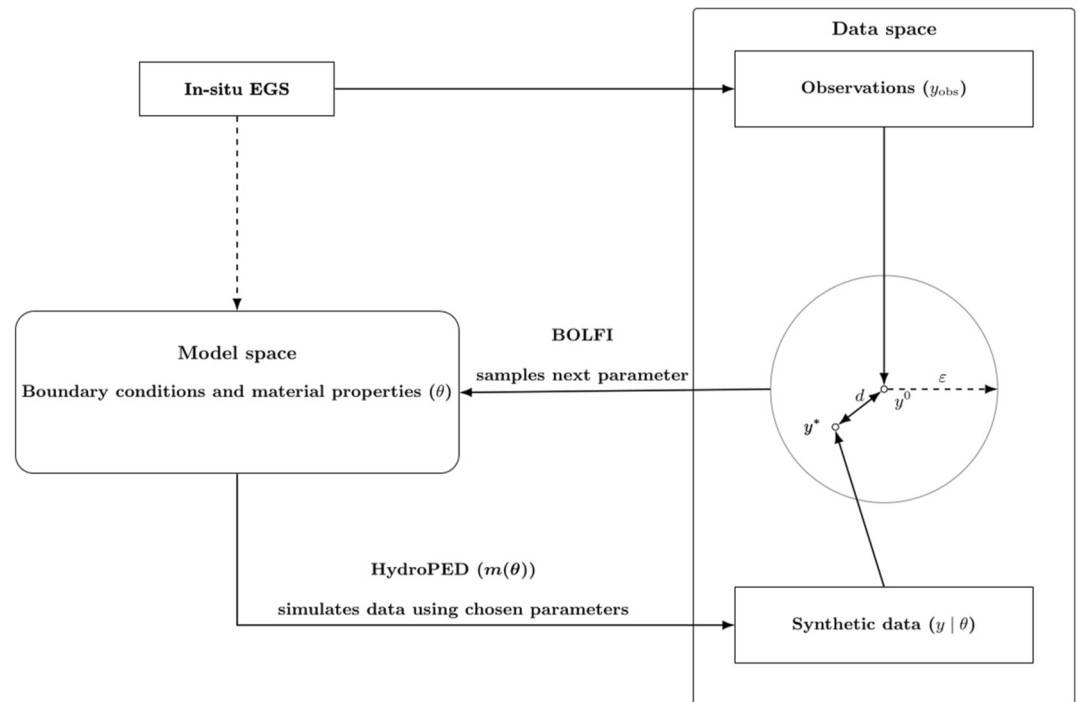


Figure 1. Workflow and key components of the inference scheme. Arrows indicate various dependencies within the computational framework. The vector of parameters that is inverted for is θ , $m(\theta)$ is the mathematical or numerical HydroPED engine that simulates synthetic data, $y|\theta$ is the simulated output governed by the parameters θ , and y^* is the processed summary statistics from these synthetics. The target observations associated with the ground truth state are y_{obs} , and y^0 is the corresponding processed summary statistic for these observations. The computed discrepancy between observed y^0 and modeled y^* summary statistics is d , and ϵ is a threshold that is dynamically updated by the Bayesian optimization for likelihood-free inference algorithm as the inversion proceeds.

observations to the local reservoir scale can be biased because of the typically incomplete knowledge of the structural heterogeneity. We demonstrate how ambient stress magnitudes can be estimated from induced seismicity data obtained from hydraulic stimulation experiments using BOLFI. We show how the selection of seismic observations and summary statistics from earthquakes influences the performance of the inversion process. The results and observations can inform future applications of the framework for the inversion of a wide range of potentially time and space dependent geothermal reservoir parameters based on the selection of appropriate target functions.

The paper is organized into five sections including the mathematical and numerical formulation of the forward damage rheology model (Section 2), the introduction to simulator-based inference and the BOLFI method (Section 3), the synthetic seismicity generation and introduction of the two tested summary statistics event count and potency (Section 4), and the inversion results using these two different statistics (Section 5). We discuss the implications of our results more broadly for the parameter estimation in complex, non-linear geophysical systems (Section 6).

2. The Damage Rheology Model

This section introduces the mathematical and numerical basis of the HydroPED simulation software. It controls the data generation part in the inference loop illustrated in Figure 1. HydroPED has been applied to various geoscience and geotechnical problems including borehole breakouts, stable and unstable damage in fracturing granites, and the effect of strain localization and the Kaiser effect on the evolution of the yield surface of brittle rocks (Gajst et al., 2020; Hamiel et al., 2006; Shalev et al., 2021). We apply HydroPED here to perform coupled seismo-hydromechanical modeling of an enhanced geothermal reservoir. While we provide an overview of how HydroPED works in this paper, the reader is encouraged to consult Lyakhovsky (1990) and Shalev and

Lyakhovsky (2013) about the theoretical and observational background of viscoelastic damage rheology, which forms the basis of HydroPED.

2.1. Review of Damage Rheology Modeling

The nonlinear behavior of rocks undergoing damage, governed mainly by dilatancy and by changes in elastic properties in response to damage accumulation in the deforming rock, has been widely observed in a number of field and experimental studies (Hamiel et al., 2011; Lockner & Byerlee, 1980; Lyakhovsky, Reches, et al., 1997). Classical models such as the Murnaghan model incorporate nonlinearity by including higher-order terms in the strain energy function (Panteleev et al., 2021). These classical nonlinear models usually predict failure prematurely and are not capable of accounting for abrupt changes upon stress reversal (Hamiel et al., 2011).

The non-classical nonlinear model implemented in HydroPED accounts for the behavior of rocks under high stresses and stress reversal on the basis of a micro-mechanical model with non-interacting randomly oriented cracks within a homogeneous rock matrix (Lyakhovsky & Myasnikov, 1984). This is achieved using one additional non-Hookean second-order term with modulus γ , which couples shear and volumetric strain, in the strain energy function F in Equation 1. HydroPED, as outlined in Figure 1, models hydraulic stimulation via fluid injection using non-classical nonlinearity integrated in a continuum damage framework (Kachanov, 1987; Lyakhovsky, Reches, et al., 1997). It uses the Explicit Finite Difference Lagrangian Method for solid deformation and the Finite Element Method for fluid conservation to solve coupled equations of poroelastic deformation, fluid pressure diffusion, and damage evolution critical in EGS (Shalev & Lyakhovsky, 2013). HydroPED uses a scalar damage variable α_D to represent local crack density which indicates the modulus reduction of an ideal fracture-free solid (Lyakhovsky & Ben-Zion, 2008; Shalev & Lyakhovsky, 2013).

2.2. General Model Formulation and Implementation

The HydroPED model involves the strain energy function F that characterizes the elastic potential of a damaged rock (Lyakhovsky et al., 2016)

$$F = \frac{\lambda(\alpha_D, \varphi)}{2} I_1^2 + \mu(\alpha_D, \varphi) I_2 - \gamma(\alpha_D, \varphi) I_1 \sqrt{I_2} + \frac{1}{2} M [\alpha_B I_1 - \zeta + \varphi]^2, \quad (1)$$

where λ and μ are the Lamé parameters of linear Hookean elasticity, $I_1 = \varepsilon_{kk}$ and $I_2 = \varepsilon_{ij}\varepsilon_{ij}$ are the first and second strain invariants, respectively, γ is a third modulus for a damaged solid, ζ is the fluid content, φ is the porosity, and M and α_B are Biot's coefficients and α_D is the damage state variable. Here, ζ is treated as a state variable representing the fluid content, that is, the increment of fluid volume per bulk expressed in the same form as porosity in the poroelastic formulation. The fluid pressure in the system is described by the negative of the term $M[\alpha_B I_1 - \zeta + \varphi]$. The constitutive relation, characterized by the stress and strain tensors (Hamiel, Liu, et al., 2004), is

$$\sigma_{ij} = \frac{\partial F}{\partial \varepsilon_{ij}} = \left(\lambda I_1 - \gamma \sqrt{I_2} \right) \delta_{ij} + \left(2\mu - \gamma \frac{I_1}{\sqrt{I_2}} \right) \varepsilon_{ij} - \alpha_B p \delta_{ij}, \quad (2)$$

where F is the strain energy function from Equation 1, p is the pore pressure, σ_{ij} is the stress tensor, ε_{ij} is the strain tensor, and δ_{ij} is the Kronecker delta. Following the standard implementation of the non-classical damage rheology formulation in HydroPED, we treat the first Lamé's constant λ as damage-independent (Hamiel et al., 2011)

$$\lambda = \text{const.}, \quad (3)$$

hence the value of λ does not change in response to variations in the damage state of the rock. The two other moduli that are damage-dependent are

$$\mu = \mu_0 + \gamma_r \xi_0 \alpha_D \quad (4)$$

and

$$\gamma = \gamma_r \alpha_D, \quad (5)$$

where μ_0 is the initial shear modulus of the intact rock, γ_r is a scaling constant that determines the values of the moduli at maximum damage, and ξ_0 is a threshold beyond which damage increases. HydroPED includes a damage kinematic component described as

$$\frac{d\alpha_D}{dt} = \begin{cases} C_d I_2 (\xi - \xi_0) & \text{for } \xi > \xi_0 \\ C_1 \exp\left(\frac{\alpha_D}{C_2}\right) I_2 (\xi - \xi_0) & \text{for } \xi < \xi_0, \end{cases} \quad (6)$$

where C_d is the rate of material degradation and C_1 and C_2 are parameters that modulate material healing. The strain invariant ratio $\xi = I_1/\sqrt{I_2}$ is a dimensionless measure of the relative contribution of volumetric strain I_1 to the shear deformation $\sqrt{I_2}$; it controls the transition between dilatant damage growth and healing in the damage rheology model. The governing fluid flow is characterized by a pressure diffusion term and a permeability-damage term. The pressure diffusion is described as

$$\nabla \cdot \left(\frac{k(\alpha_D)}{\mu_f} (\nabla p + \rho g z) \right) = S_e \frac{\partial p}{\partial t} + \alpha_B \frac{\partial \epsilon_{kk}}{\partial t}, \quad (7)$$

where $k(\alpha_D)$ is the damage-dependent permeability of the medium, μ_f is fluid viscosity, ρ is fluid density, g is acceleration due to gravity, S_e is specific storage, and z is a unit vector in the vertical direction. The permeability damage term is

$$k(\alpha_D) = k_0 \exp(b\alpha_D), \quad (8)$$

where k_0 is the initial permeability tensor and b is a permeability enhancing damage parameter.

HydroPED consists of two coupled main modules. The mechanical module handles solid deformation and seismicity by solving the equation for strain energy (Equation 1), the constitutive relations (Equations 2–5), and damage evolution (Equation 6). The fluid flow module addresses pressure diffusion and permeability changes by solving Equations 7 and 8, respectively. An optional third heat module simulates conductive and convective temperature changes but is excluded here due to short simulation times on the order of one day, where mechanical and hydrological changes dominate (Levin et al., 2020). Detailed module descriptions are provided in Appendices A and B.

2.3. Seismicity and Damage Modeling

HydroPED links seismicity to continuum damage evolution. When the damage variable α_D reaches a critical level, the strain energy function loses convexity and an event is triggered. In practice, an event corresponds to a stress-drop episode on one or more elements within a time step with the involved elements defining the effective rupture area, and the simulator records the corresponding catalog entry. Events are represented by a Drucker–Prager stress-drop formulation, which yields elastic energy release with permanent plastic strain (Lyakhovsky, Reches, et al., 1997; Shalev & Lyakhovsky, 2013). Tensile and shear failure conditions are then evaluated using the strain invariant ratio ξ . Tensile failure is described by

$$2\mu - \gamma\xi = 2\mu^e \geq 0, \quad (9)$$

where $\mu^e = \mu - \gamma\xi/2$ (Lyakhovsky, Ben-Zion, & Agnon, 1997). Shear failure is modeled by slip across surfaces or faults that result from elevated damage levels under compressive loading conditions described by

$$(2\mu - \gamma\xi)^2 + (2\mu - \gamma\xi)(3\lambda - \gamma\xi) + (\lambda\gamma\xi - \gamma^2)(3 - \xi^2) \geq 0, \quad (10)$$

Table 1
Selected Material Properties Used in the HydroPED Forward Simulations

Material property	Range	Value used	Reason	Equation
Density, ρ [kg/m ³]	2.5e3–4.0e3	2.7e3	A typical value for the density of granite in the crust	Equation A2
Young's modulus, E [Pa]	30.0e9–50.0e9	40.0e9	Average value from field and laboratory experiments	Equations 1 and 2
Poisson ratio, ν [–]	0.15–0.25	0.2	A lower than typical value to account for reduced stiffness associated with cracks or initial damage	Equation 2
Biot modulus, M [Pa]	10.0e9–50.0e9	15.0e9	Estimated value using a 2 GPa bulk modulus of water and a total pore space of 12.5% (10% average element damage and 2.5% rock matrix porosity)	Equation 1
Critical strain-invariant ratio, ξ_0 [–]	–0.7–1	–0.95	Damage must reach a higher value before seismicity occurs	Equation 4
Damage rate parameter, C_d [–]	2.5e3–3.5e3	3.0e3	Support faster rates of damage accumulation	Equation 6
Healing rate parameter 1, C_1 [–]	1.0e–24–1.0e–4	1.0e–5	Support faster rates of healing	Equation 6
Healing rate parameter 2, C_2 [–]	0.01–0.04	0.03	Support faster rates of healing	Equation 6
Dynamic weakening parameter, τ_d [s]	1.0–1.0e4	3.0	This produces seismic events of similar sizes. Larger values yield events with wider range of sizes	Equation 11
Initial damage, α_D [–]	0.0–0.6	0.2	Limits the initial damage in each element to 20%	Equations 4–8
Amplitude of random noise, A_n [–]	0.05–0.15	0.1	Controls the ~10% random variation in initial damage value for each element	Equations 4–8
Coefficient of damage related viscosity, C_v [1/Pa]	1.0e–12–1.0e–10	1.0e–11	Yields moderate levels of viscosity from damage accumulation	Equation A3
Initial permeability, k_0 [m ²]	3.0e–19–3.0e–14	3.0e–17	Typical value for unfractured granite	Equation 8
Permeability growth factor, b [–]	10–20	16	Accounts for moderate permeability growth due to damage accumulation	Equation 8
Biot coefficient, α_B [–]	0–1	1	$K_b \ll K_s$, where K_b is the bulk modulus of the drained rock matrix and K_s is the bulk modulus of the solid grains, has almost all the applied stress transferred to the fluid because $\alpha_B = 1 - \frac{K_b}{K_s}$	Equations 1 and 7

where all the terms described in Equations 9 and 10 retain their meanings as previously defined (Lyakhovsky, Ben-Zion, & Agnon, 1997). The Drucker–Prager formulation links rupture area to seismic potency (a scalar measure proportional to slip area times average slip) and has been calibrated using typical stress-drop and friction ranges (Lyakhovsky, Reches, et al., 1997). After an event, slip terminates and healing proceeds according to Equation 6, with dynamic healing represented by

$$\alpha_D = \alpha_c - \sqrt{\tau_d \frac{d\alpha}{dt}}, \quad (11)$$

where τ_d is the characteristic timescale for seismic wave damping in an undamaged material and α_c is the critical damage level defined by Equations 9 and 10 (Finzi, 2010). A more comprehensive description of the seismic modeling approach can be found in Shalev and Lyakhovsky (2013).

The damage model parameters C_d , C_1 , and C_2 (Equation 6) control the geometry of evolving faults, seismicity patterns, and the spatiotemporal distribution of deformation (Finzi, 2010). Damage accumulation is mainly governed by C_d , healing by C_1 and C_2 , and brittleness by the initial damage level (Lyakhovsky et al., 2001). Additional parameters include ξ_0 , C_v , and the damping timescale τ_d . These and other model parameters and material properties used in this study are summarized in Table 1.

2.4. Mesh Generation and Pre-Processing

The computational domain for the forward solver is a cube with a length of 2 km meshed using the open-source meshing tool Gmsh to produce tetrahedral meshes using the Delaunay algorithm. The meshed domain used in this

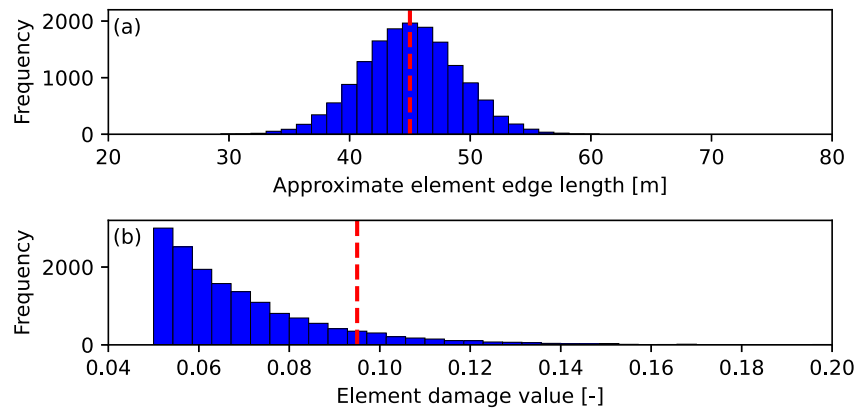


Figure 2. Properties of the computational mesh. (a) Distribution of element sizes. (b) Distribution of the initial damage parameter α_D . The red dashed lines indicate the mean of each distribution.

study has 15,787 tetrahedral elements and 3,394 nodes, including 1,624 boundary nodes. The size of the element follows a Gaussian distribution with an approximate average edge length of 45 m (Figure 2a). Pre-processing involves creating the inventory that stores the element information, the nodes and their corresponding coordinates, the connections between the nodes and the elements, boundary nodes and their corresponding boundary conditions, and defining the location of the injection point.

An important pre-processing step is the implementation of the initial damage distribution for the elements. Here, the initial damage distribution across the computational domain follows a power-law distribution (Figure 2b), parameterized by a lower and upper bound and an exponent chosen to reflect a reasonable fracture-length statistics in the rock mass. In the current implementation, initial damage values are sampled independently for each element, that is, without imposing an explicit spatial correlation. Each forward simulation is governed by a different realization of this random damage field while preserving the same power-law statistics. The resulting variability introduces an irreducible component of simulator uncertainty, which is handled in the likelihood-free inversion by treating the discrepancy as a stochastic function of θ and learning it with the Gaussian-process surrogate.

The power-law damage distribution affects the frequency-size (FS) statistics of the simulated earthquake response. This is well understood from numerous studies that established a relation between computational tuning parameters reflecting length and size scale distributions in earthquake simulators and the system response (Ben-Zion, 2008). It is appealing to utilize the FS statistics as a target function in our inversion approach, considering that properties of the FS statistics including the b-value are indicative of the stress regime (Schorlemmer et al., 2005). However, the effects of the random initial damage distribution and the HydroPED damage model parameters C_d , C_1 , and C_2 , as well as τ_d discussed in Section 2.3 have to be explored in more detail before we can use the FS statistics as effective target function.

2.5. Simulation Products

The simulator computes the spatio-temporal evolution of state variables, including damage distribution, fluid pressure, shear stress, rock pressure, and other non-state variables such as the permeability or the flux through the injection point, and it also compiles a synthetic seismicity catalog. Figure 3 shows an example fluid pressure pattern and the corresponding damage distribution for a simulation obtained with HydroPED. The damage distribution is consistent with the expected behavior where damage accumulates along the maximum horizontal stress, here along the horizontal y direction. Hence, the damage zone elongates with increasing time. The fluid pressure field is also compatible with the expectation that an exponentially decaying pressure front is observed away from the injection point. The fluid pressure front shows a consistent, yet irregular dependence on the distance to the central injection point, where the irregularity is associated with the grid element size and geometry, and the seeded element damage.

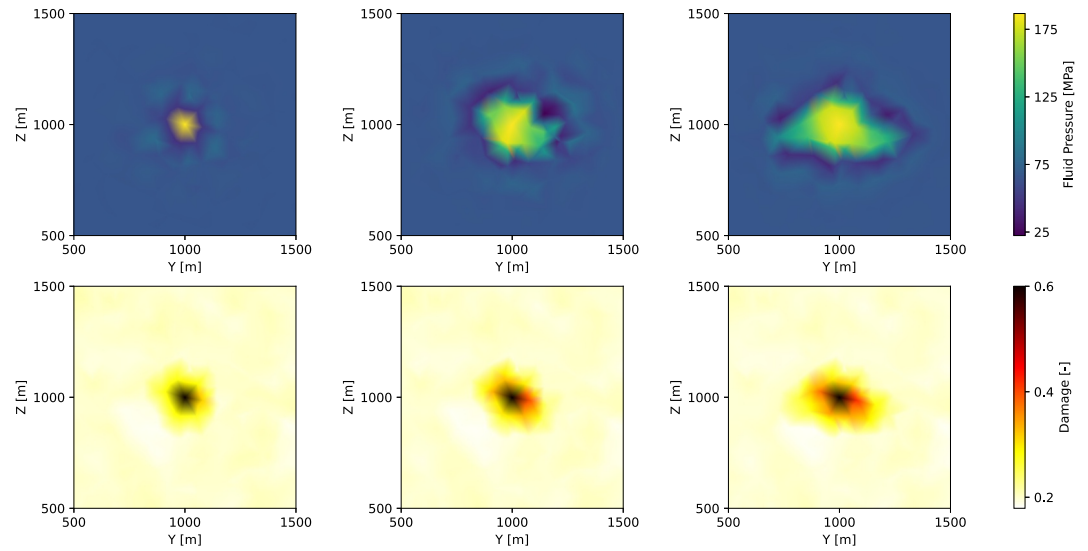


Figure 3. HydroPED output showing 2D distributions of the fluid pressure and the damage variable in response to an injection after 1, 3, and 6 days in the y - z plane. The stress parameters used for this simulation are $\sigma_H = 240$ MPa, $\sigma_v = 180$ MPa, $\sigma_h = 140$ MPa, and $\sigma_p = 120$ MPa. The fluid pressure field decays exponentially away from the injection point, and the damage field elongates in the same direction as the fluid pressure field. The maximum principal stress acts along the y direction and controls the elongated shapes of the patterns in this direction.

3. Simulator-Based Inference

This section summarizes the simulator-based inference (SBI) workflow used in this study as shown in Figure 1. This follows a standard inversion workflow where a posterior distribution $p(\theta|X_{\text{obs}})$ is estimated using a forward simulator that does not provide a tractable likelihood $p(X|\theta)$ but can only generate synthetic observations for a given parameter vector θ (Lueckmann et al., 2021).

We infer a posterior over the reservoir parameters using summary features extracted from some relevant data sources. In EGS applications, a likely data source is observations that are typically collected in seismicity catalogs. This can be first order estimates of timing, location, event magnitude, or more detailed information about the focal mechanisms, but also other seismic observables indicative of the medium variations such as changes in the P wave speed to S wave speed ratio, or estimates associated with an increased medium heterogeneity characterized by the scattering cross section obtained from passive monitoring (Hillers et al., 2015). Examples of these data sources include earthquake b -values, seismogenic index, spatial release of energy or potency, and the spatial hypocenter distribution (Shapiro, 2018).

Some SBI methods include ABC and BOLFI. ABC in its basic form, rejection-ABC, samples candidate parameters from a given prior distribution $p(\theta)$ and accepts candidate parameters when the discrepancy between observed and simulated summaries is below a tolerance ϵ . BOLFI is a model-based ABC method which uses an active learning framework to learn a surrogate model of the discrepancy using an acquisition rule to choose the next parameter values to simulate (Gutmann & Corander, 2016). The key novelty in this study is coupling BOLFI to HydroPED to obtain informative posteriors for a complex, quasi-stochastic system with very few simulator evaluations. Accordingly, we provide more details about the BOLFI algorithm.

3.1. Bayesian Optimization for Likelihood-Free Inference (BOLFI)

The BOLFI algorithm sketched in Appendix D is used to perform parameter inversion as shown in Figure 1. It improves on rejection-ABC by approximating an effective likelihood $p(s(X_{\text{obs}})|\theta)$ with a statistical model and by using acquisition rules to efficiently minimize the discrepancy Δ_θ (Aushev et al., 2022; Gutmann & Corander, 2016). In this study we use the logarithm of the L2 norm as the discrepancy measure,

$$\Delta_{\theta} = \log \|\mathbf{T} - \mathbf{S}\|_2 = \log \sqrt{\sum_{i=1}^n (T_i - S_i)^2}, \quad (12)$$

where T is the target data vector, S is the synthetic data vector, and n indicates the number of observations. Taking the logarithm reduces the dynamic range of discrepancies and helps balance contributions when summary components differ in scale, which stabilizes the Gaussian-process fit and the acquisition optimization. We treat Δ_{θ} as a stochastic function of θ and model it with a Gaussian-process (GP) surrogate,

$$\Delta_{\theta} \approx GP(m(\theta), k(\theta, \theta')), \quad (13)$$

where we assume the function mean $m(\theta) = 0$. We standardize the observed discrepancy values by subtracting their sample mean and scaling by their sample standard deviation for the current design, so that the deviations of the GP models are about a centered baseline and ensure the model makes no prior assumptions about the trend of the function unless data is observed. The covariance is given by

$$k(\theta, \theta') = \sigma_{\Delta_{\theta}}^2 \exp \left(\sum_j \frac{1}{\lambda_j^2} (\theta_j - \theta'_j)^2 \right), \quad (14)$$

where λ_j is a length scale hyperparameter and $\sigma_{\Delta_{\theta}}^2$ is the discrepancy variance (Gutmann & Corander, 2016).

BOLFI selects the next ambient stress values using an acquisition rule that improves the surrogate in Equation 13. We use the maxvar acquisition rule, which targets regions where posterior uncertainty is largest (Figure 4); its formulation is summarized in Appendix C. Maxvar supports parallel sampling without updating the GP between batches, and we adopt it to efficiently explore stress values that reproduce the target seismicity features (Järvenpää et al., 2019). The BOLFI algorithm is run for 200 and 500 iterations, and the results are collected as a set of parameter values θ that are approximate samples from the posterior distribution $p(\theta|X)$. These samples can be used for computing statistics, for visualizing the posterior, or for running further simulations. Details of the BOLFI algorithm can be found in Algorithm 1.

4. Simulated Data

4.1. The Model Set Up

We use simulated data to validate the usefulness of BOLFI in likelihood-free inference for EGS parameter estimation because the ground truth parameters are known and the impact of target function choice and evidence count can be assessed without additional observational uncertainty. We define a synthetic target catalog generated with HydroPED to provide a controlled reference case for stress inversion. We use a synthetic target catalog generated with HydroPED using principal stress values that are informed by the 6 km deep geothermal reservoir in the Helsinki area, Finland. In 2018 and 2020, two weeks-long stimulations of the Fennoscandian Shield bedrock resulted in abundant induced seismicity, where the largest event had a local magnitude of $M_L 1.8$ (Kwiatek et al., 2019). Kwiatek et al. (2019) estimated the ambient principal stress values as $\sigma_H = 240$ MPa, $\sigma_v = 180$ MPa, and $\sigma_h = 110$ MPa. Our simulated ground truth values in this study are $\sigma_H = 250$ MPa, $\sigma_v = 160$ MPa, $\sigma_h = 100$ MPa, and $\sigma_p = 105$ MPa. These values are chosen close to the estimated ground truth values from Kwiatek et al. (2019) but adapted to generate a statistically large number of events. The cubic computational domain is characterized by homogeneous conditions except for the randomly varying initial damage values. It contains a single injection point at the center where we apply a constant injection pressure. We use a fixed boundary condition with zero deformation at the boundaries. This setup is used to infer ambient principal stresses in the reservoir with BOLFI using data obtained from simulated earthquake catalogs. The average wall-clock time for one forward execution of HydroPED for this study on a 2.40 GHz Intel Xeon E5-2630 v3 (Haswell) with an 8-core CPU node with 192 GB of DDR4 RAM is approximately 1.5 hr; this timing is hardware-dependent. Each forward simulation computes the response to one day of stimulation.

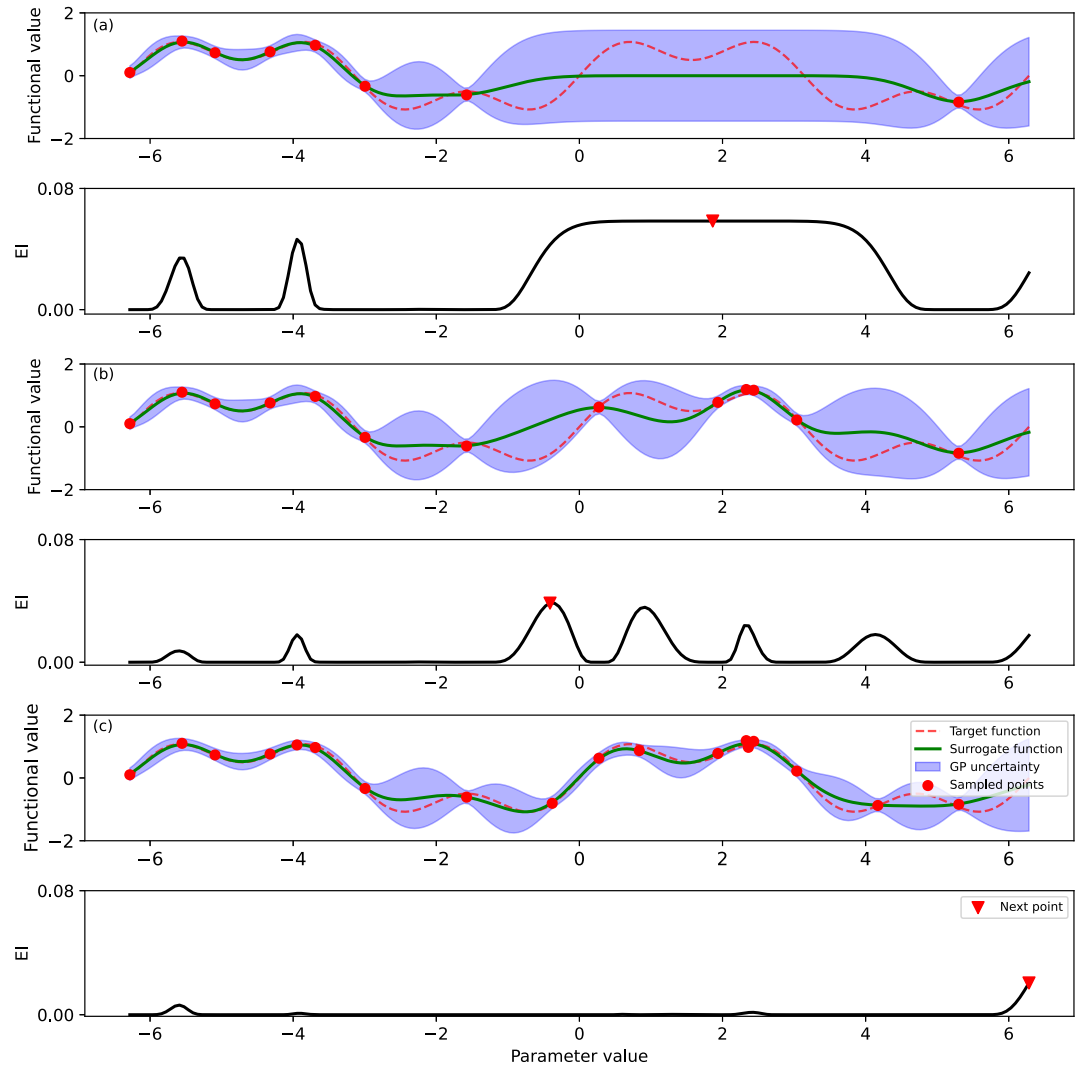


Figure 4. Conceptual representation of the Bayesian optimization for likelihood-free inference (BOLFI) inversion after (a) 8, (b) 13, and (c) 18 evidences. The evidences are simulated data given to BOLFI to build a surrogate model. In all cases three initial observations are provided. The number of evidences include both the initial data fit and the subsequent number of forward evidences. The top panel in each subplot shows the red indicated target function, the Gaussian Process GP uncertainty associated with the green indicated estimate or surrogate model, and the parameter value that is sampled to constrain the target function. The surrogate model represents the estimate that BOLFI builds for the underlying target function. The lower panel in each subplot shows the acquisition function or the Expected Improvement EI that tells the algorithm which parameter value should be sampled on the next iteration. Note the higher uncertainty in regions with lower sample density.

4.2. Summary Statistics

We extract two summary statistics from the simulated catalogs and use them as separate targets for principal stress inference. The first is a vector of event counts in each of eight Cartesian quadrants centered at the injection location, plus the total event count (Figure 5a). We use eight quadrants as a simple, low-dimensional partition that preserves coarse 3D spatial information while keeping the summary dimension small enough for inference under limited simulator budgets. The second is a vector of total event potency in each quadrant plus the total potency in the system (Figure 5b). Unless stated otherwise, these summary vectors are used without additional normalization or weighting beyond the discrepancy definition in Equation 12. The scalar potency value P of a seismic event is

$$P = Au, \quad (15)$$

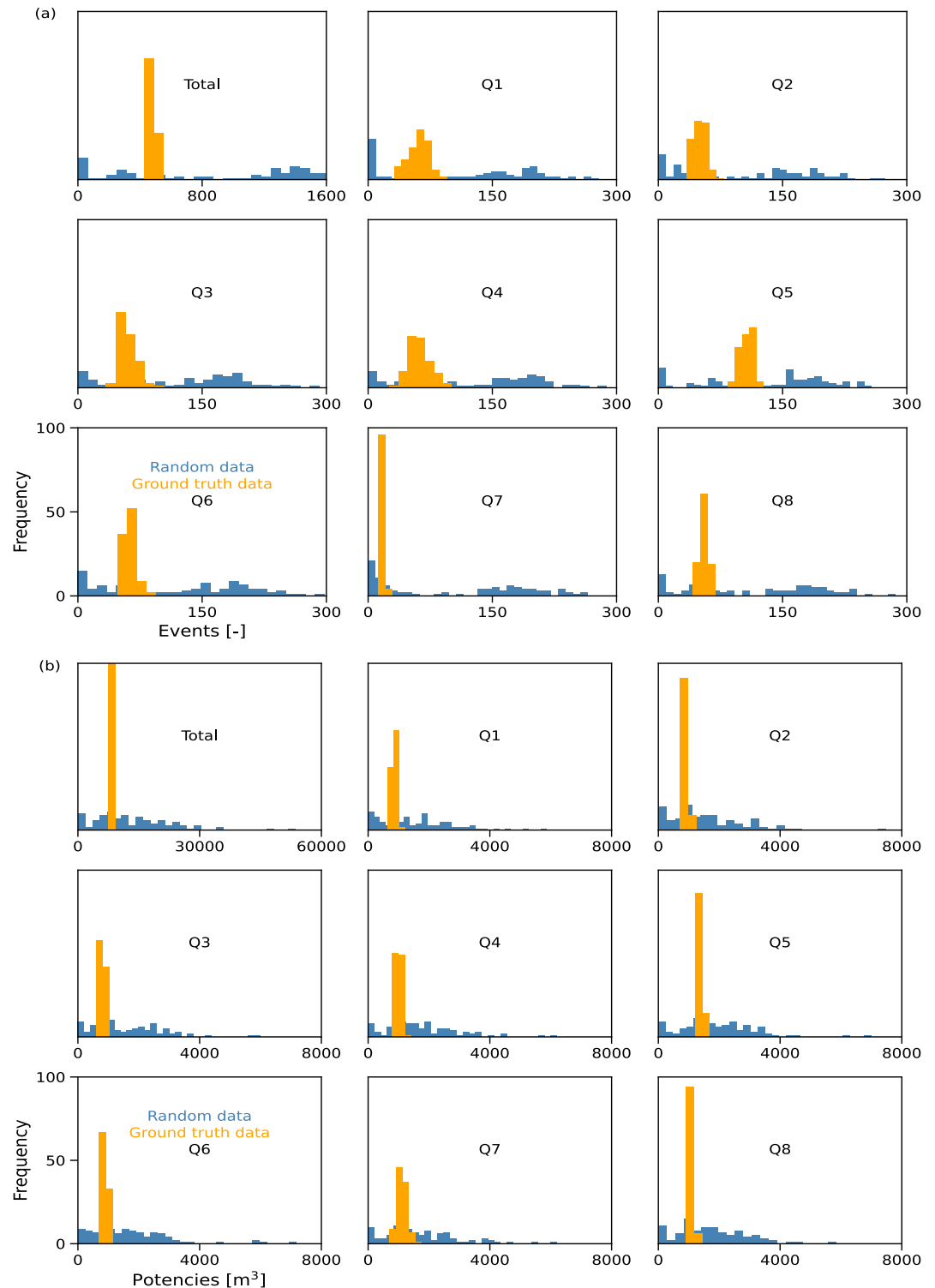


Figure 5. The two different summary statistics explored in this work. (a) The summary statistics for the event count target function. (b) The summary statistics for the potency target function. Q1 to Q8 indicate the statistics in the eight quadrants about the injection, and “Total” considers the full domain. The blue distributions are obtained from simulations with randomly chosen stress and pressure values. The orange distributions are obtained from our ground truth simulations. All panels have the same y-axis range.

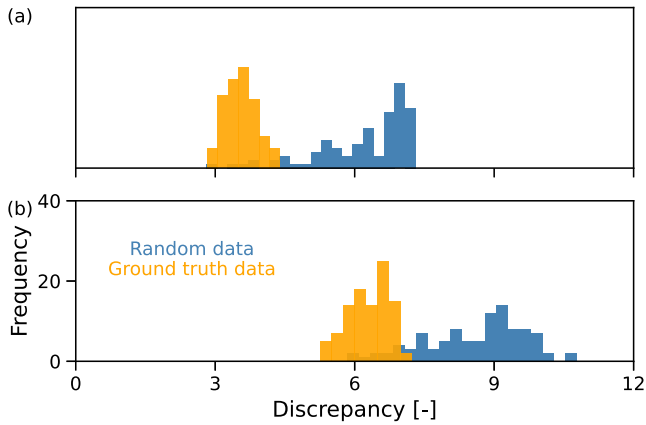


Figure 6. Discrepancy summary statistics results for (a) the event count target function and (b) the potency target function. The blue distributions are obtained from simulations with randomly chosen stress and pressure values. The orange distributions are obtained from our ground truth simulations. All panels have the same y-axis range.

where A is the cross-section area of slip and u is the slip length. The tensor representation of potency is

$$P_{ij} = \int_v \Delta \epsilon_{ij}, \quad (16)$$

where $\Delta \epsilon_{ij}$ is the strain in a deforming element with volume v . The total potency P_T is then represented as the Frobenius norm

$$P_T = \|P_{ij}\| = \sqrt{\sum \Delta \epsilon_{kk}^2 + 2(\sum \Delta \epsilon_{ij}^2)}, \quad (17)$$

with $i \neq j$.

Figure 6 shows discrepancy distributions (Equation 12) for event count (top) and potency (bottom) targets. Colors indicate two sampling strategies: always using the synthetic ground-truth stresses (orange) versus stress values drawn from the priors (blue). The finite width for the ground-truth case and consistent lower bounds in both cases are governed by the random initial damage distribution and provide an inherent resolution limit. The discrepancy ranges vary due to the scales of the underlying metrics.

4.3. Sensitivity of Summary Statistics to Model Parameters

We perform a sensitivity analysis of the synthetic catalogs to evaluate how σ_H , σ_v , σ_h , and σ_p affect the potency summary statistic and how well BOLFI can constrain these stresses when potency is the target. Figure 7 shows the relationship between each ambient stress component and the corresponding potency response. Each panel shows three potency curves where red, blue, and green correspond to low, median, and high prior values of the remaining stress components, respectively. For each curve, the stress component on the x-axis is varied while the other stress components are held fixed. Figure 7 shows a strongly nonlinear and non-monotonic dependence of total potency on the stress components. The response is most sensitive to changes in the horizontal stresses σ_H and σ_h , whereas σ_v and σ_p have weaker and more scattered effects over their prior ranges. This level of nonlinearity shows that the underlying inverse problem is a very complicated one and would require more sophisticated methods to extract meaningful inversion results.

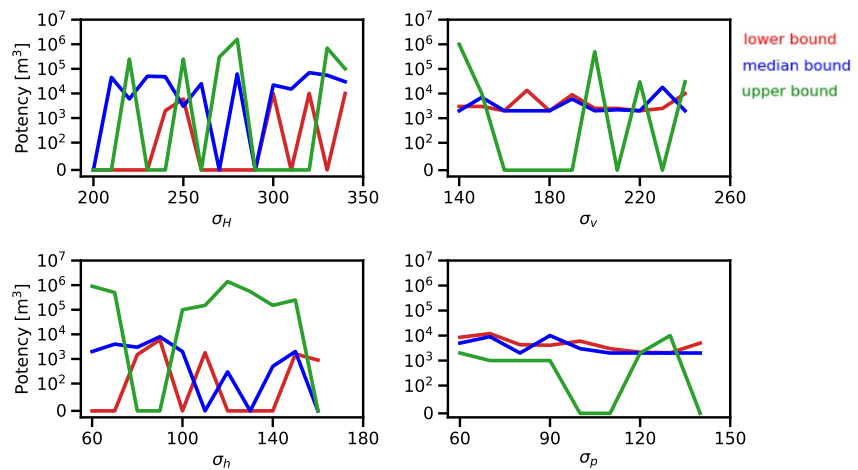


Figure 7. Stress parameter sensitivity test results using potency summary statistics. Each line represents a simulation outcome where a single corresponding stress parameter is varied and the other three are fixed. The red lines indicate when the lower bound values of the priors are used. The blue lines indicate when the median values are used, and the green line indicates when the upper bound values are used. All values are in MPa.

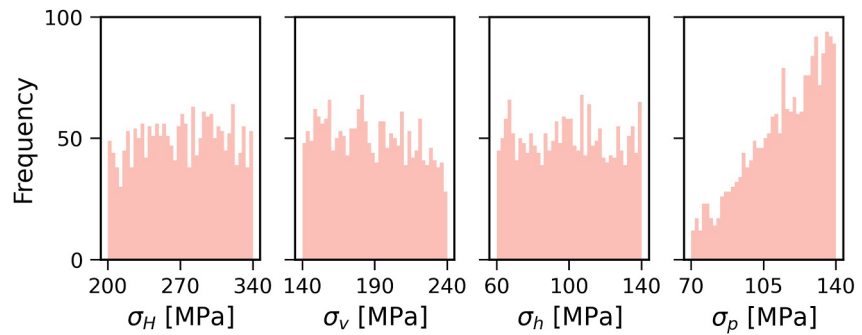


Figure 8. Prior distributions of the four stress parameters that we invert for. These distributions are reproduced in Figures 10 and 13 for comparison.

5. Results

Figure 8 shows the prior distributions of the reservoir principal stress components and the injection overpressure. The maximum horizontal stress σ_H varies uniformly between 240 and 340 MPa, with bounds estimated from the stress-depth relations for the Fennoscandian Shield and Finnish basement rock, $\sigma_H = 2.8 + 0.04z$ and $\sigma_H = 7.7 + 0.05z$, where z is the depth range 6 ± 2 km (Huhta & Korsman, 2005). The vertical stress σ_v varies uniformly between 140 and 240 MPa, with bounds obtained from $\sigma_v = \rho gz$ where ρ is the rock density from Table 1 and z is depth. The minimum horizontal stress σ_h is uniform between 60 and 140 MPa, where the lower bound is constrained by the first pressure drop value from the Helsinki injection experiment in Kukkonen et al. (2023) and the upper bound equals the lower bound value of σ_v . The lower bound of σ_p is estimated as the average pressure value from a Helsinki project injection pressure plot (Kwiatk et al., 2019), and the upper bound equals the lower bound of σ_h . The overpressure σ_p is constrained using $\sigma_p \geq 0.5(\sigma_H - \sigma_h)$ together with $\sigma_H > \sigma_v > \sigma_h$.

The BOLFI algorithm samples combinations of ambient principal stress values to minimize the misfit between observed and simulated summary statistics. We use the summary statistics in Section 4.2, event count and total potency, as target functions, and test inversions with 200 and 500 evidences or iterations, where each evidence corresponds to one forward simulation and its evaluated discrepancy. Here, we present the inversion results and analyze how target function choice and evidence count affect the inferred ambient principal stress value distributions.

The event count target function yields useful inversion results. In Figure 9a, the 200-evidence inversion produces a narrow low-discrepancy region of ambient principal stress values. The contours visualize the Gaussian-process surrogate prediction of the discrepancy surface over the shown parameter subspace corresponding to the green surrogate function and associated *GP* uncertainty shown in Figure 4, and the red points are the evaluated parameter samples used to fit and refine this surrogate. The comparatively small white region in Figure 9a suggests that 200 evidences do not sample a broad enough ensemble of parameter values to characterize uncertainty. Increasing the evidence count to 500 improves the sampling and yields a broader region of low-discrepancy values in Figure 9b, enabling improved uncertainty quantification.

The estimated minimum discrepancy stress values using 200 evidences are $\sigma_H = 270$ MPa, $\sigma_v = 190$ MPa, $\sigma_h = 100$ MPa, and $\sigma_p = 90$ MPa, and using 500 evidences yields $\sigma_H = 285$ MPa, $\sigma_v = 190$ MPa, $\sigma_h = 120$ MPa, and $\sigma_p = 140$ MPa. This indicates that the event count target function reconstructs parameter values that are significantly different from the synthetic ground truth defined in Section 4. Figure 10a shows the posterior distribution using 200 evidences with sampled posterior means of $\sigma_H = 290$ MPa, $\sigma_v = 196$ MPa, $\sigma_h = 120$ MPa, and $\sigma_p = 130$ MPa. The corresponding results obtained with 500 evidences shown in Figure 10b are $\sigma_H = 284$ MPa, $\sigma_v = 190$ MPa, $\sigma_h = 114$ MPa, and $\sigma_p = 125$ MPa.

We observe that reconstructing the effective stresses (post-injection) in Figures 11b and 11d is closer to the synthetic ground truth than reconstructing the unsaturated pre-injection stress state in Figures 11a and 11c, and that posterior mean estimates improve when the number of evidences increases from 200 to 500. This is consistent with the average deviation of estimated stresses from the ground truth.

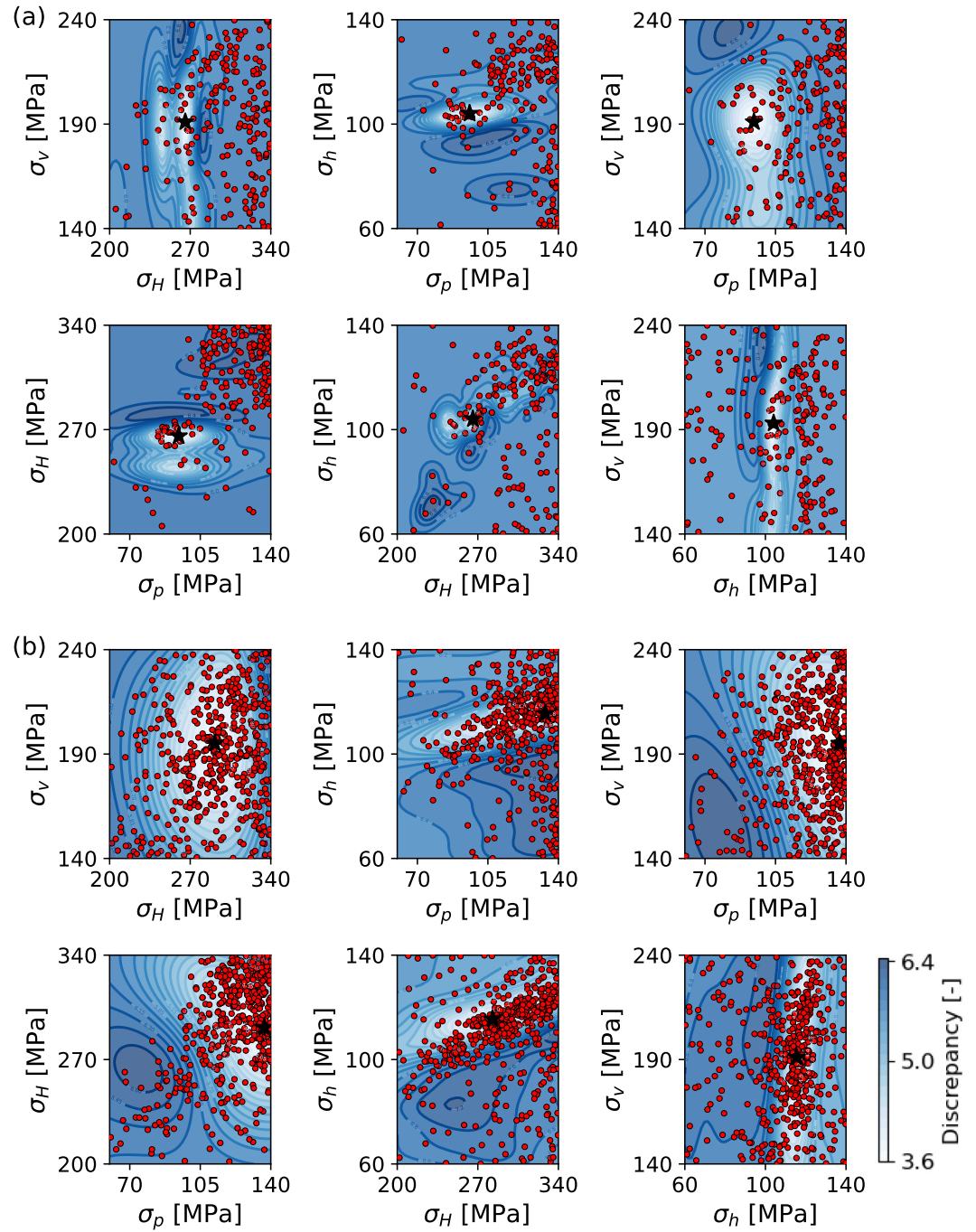


Figure 9. Inversion contour plots for the event count summaries. Results in panel (a) are obtained from 200 evidences and results in panel (b) are obtained from 500 evidences. The black star in each panel indicates the minimum discrepancy.

In contrast to the event count target function, the total potency target function yields more robust inversion results when identifying regions of minimum discrepancy in the parameter space. The values are rounded to the nearest integer. For instance, Figure 12a (200 evidences) shows minimum-discrepancy estimates $\sigma_H = 220$ MPa, $\sigma_v = 155$ MPa, $\sigma_h = 90$ MPa, and $\sigma_p = 95$ MPa, which are close to the synthetic ground truth values, and also resolves an extended zone of plausible stress values for improved uncertainty quantification. Figure 12b (500 evidences) yields minimum-discrepancy values $\sigma_H = 260$ MPa, $\sigma_v = 185$ MPa, $\sigma_h = 95$ MPa, and

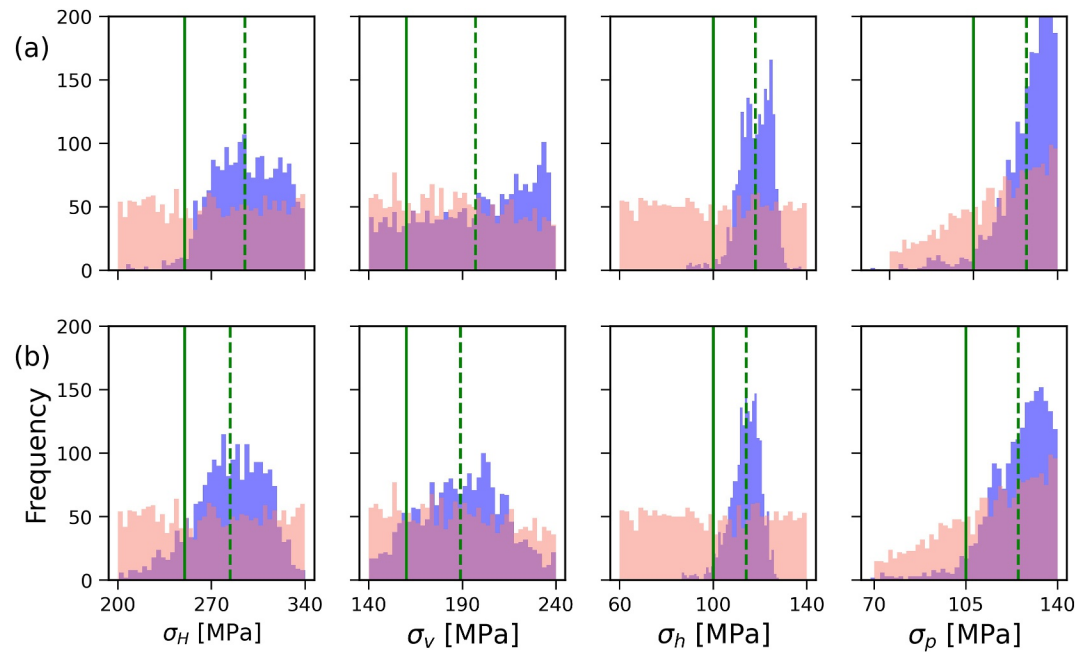


Figure 10. Sampled posterior distribution using event count summaries where (a) is obtained from inversion with 200 evidences and (b) from inversion with 500 evidences. The blue distribution is the reconstructed posterior distribution, and the light brown distribution is the prior distribution from Figure 8 for comparison. The solid green lines indicate the simulated ground truth values, and the green dashed lines show the mean posterior distribution estimates.

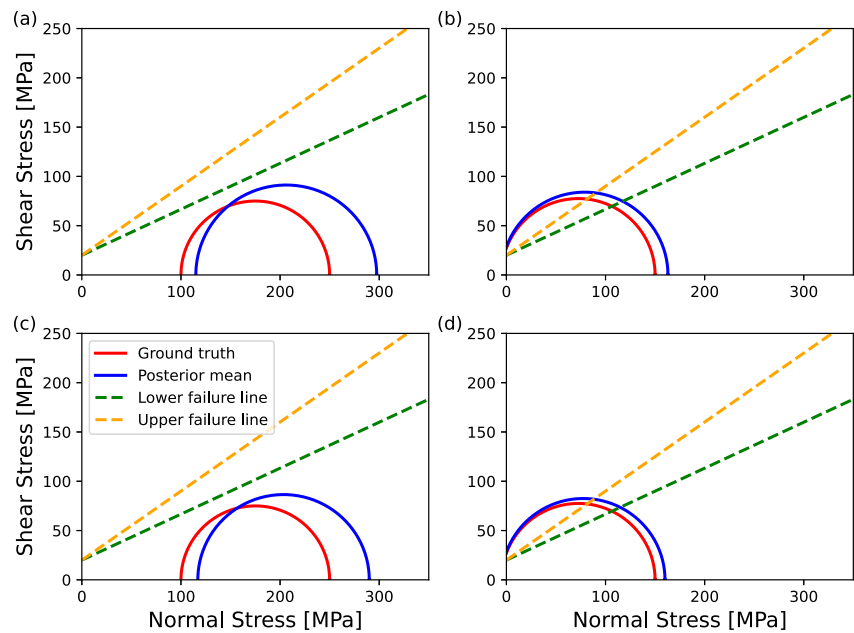


Figure 11. Mohr circle representation corresponding to the sampled posterior distribution mean values using event count summaries. The top panels (a) and (b) correspond to the stress state obtained after 200 evidences. The bottom panels (c) and (d) correspond to the stress state obtained after 500 evidences. The left panels (a) and (c) describe the pre-injection stress state. The right panels (b) and (d) describe the post-injection stress state.

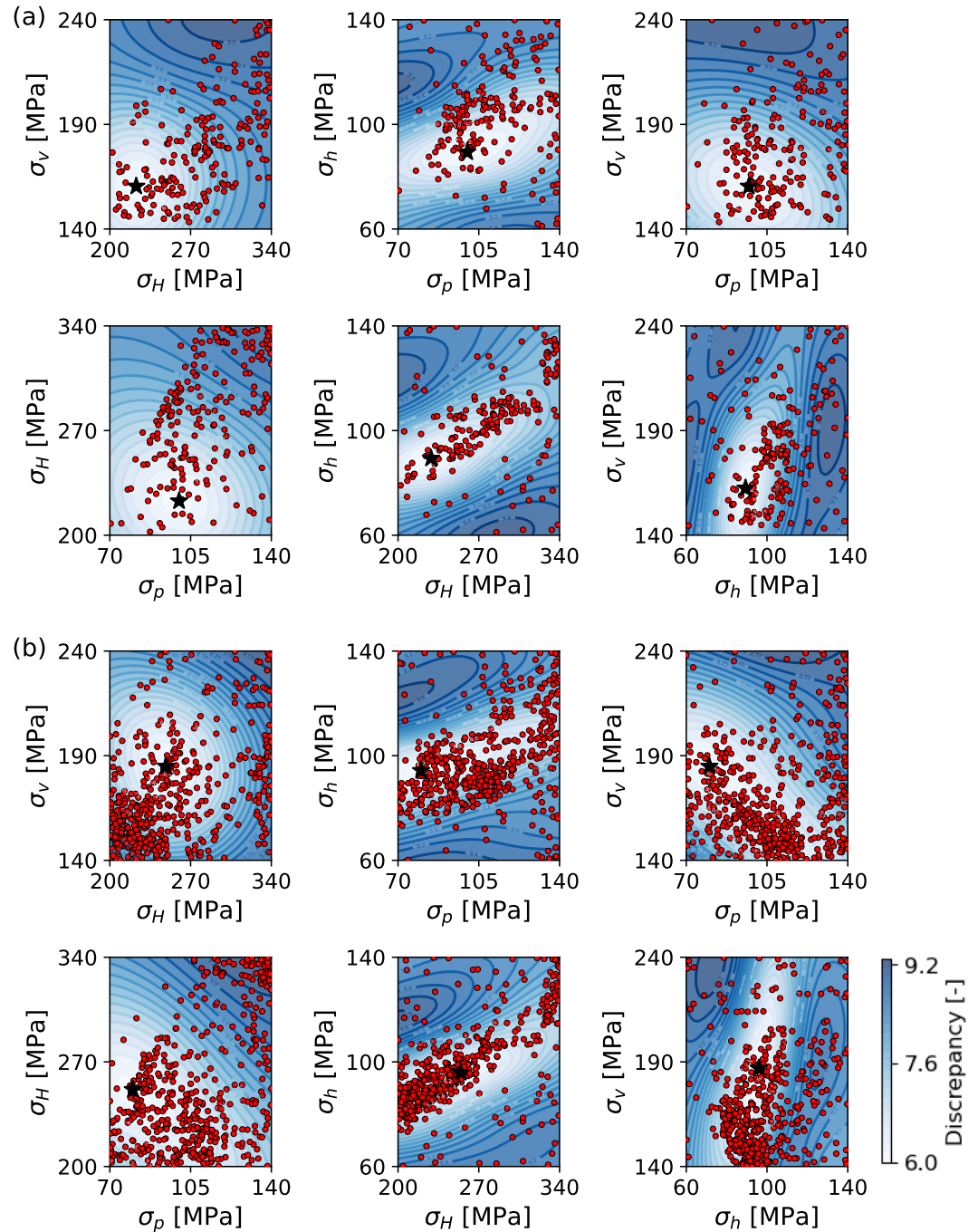


Figure 12. Inversion contour plots for the potency summaries. Results in panel (a) are obtained from 200 evidences and results in panel (b) are obtained from 500 evidences. The black star in each panel indicates the minimum discrepancy.

$\sigma_p = 80$ MPa and indicates a yet expanded low-discrepancy zone relative to Figure 12a, reflecting better-resolved trade-offs for evaluating the ambient stresses.

Figure 13a shows the posterior distribution using 200 evidences with the sampled posterior means given by $\sigma_H = 255$ MPa, $\sigma_v = 180$ MPa, $\sigma_h = 102$ MPa, and $\sigma_p = 112$ MPa. The results in Figure 13b are obtained using 500 evidences. The posterior means are $\sigma_H = 245$ MPa, $\sigma_v = 171$ MPa, $\sigma_h = 98$ MPa, and $\sigma_p = 102$ MPa. This result highlights that the spatial distribution of seismic potency release reflects the ambient stress distribution in a geothermal reservoir and is relatively robust to prior assumptions. This is well observed for

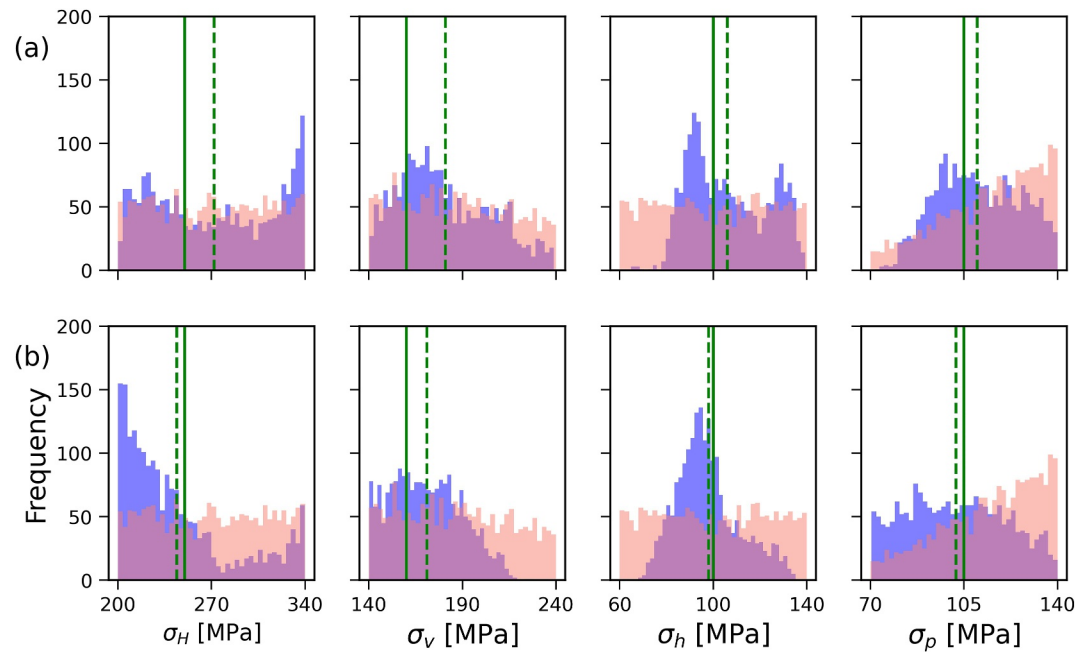


Figure 13. Sampled posterior distribution using potency summaries where (a) is obtained from inversion with 200 evidences and (b) from inversion with 500 evidences. The blue distribution is the reconstructed posterior distribution, and the light brown distribution is the prior distribution from Figure 8 for comparison. The solid green lines indicate the simulated ground truth values, and the green dashed lines show the mean posterior distribution estimates.

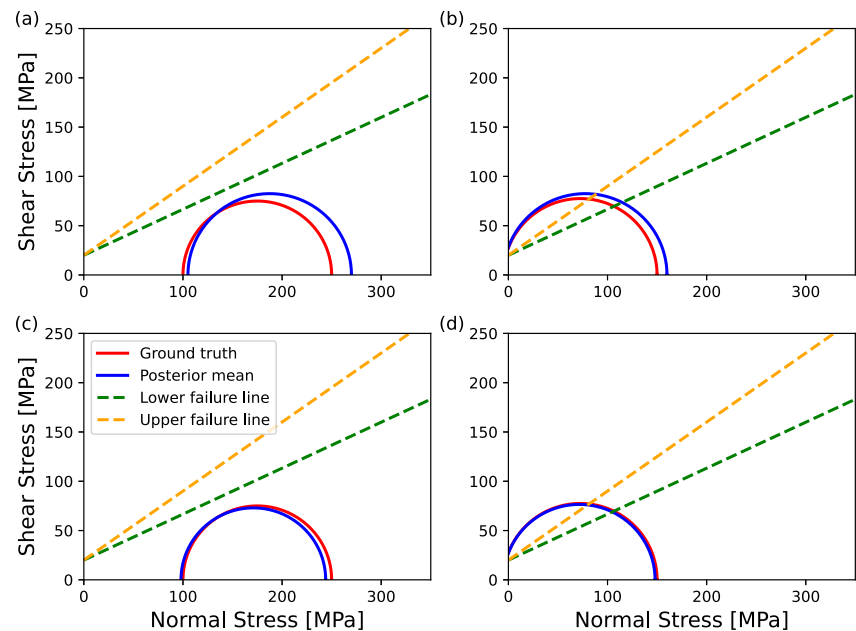


Figure 14. Mohr circle representation corresponding to the sampled posterior distribution mean values using potency summaries. The top panels (a) and (b) correspond to the stress state obtained after 200 evidences. The bottom panels (c) and (d) correspond to the stress state obtained after 500 evidences. The left panels (a) and (c) describe the pre-injection stress state. The right panels (b) and (d) describe the post-injection stress state.

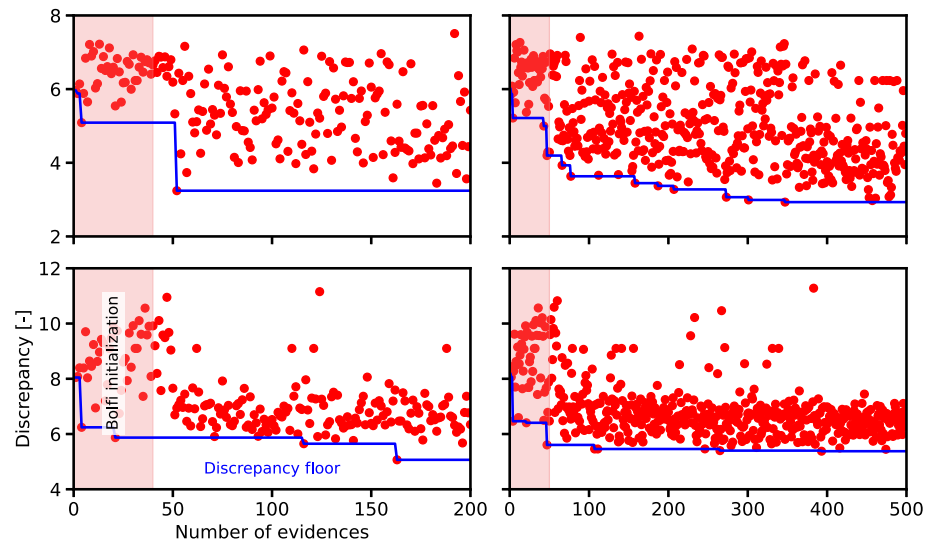


Figure 15. Evolution of the discrepancy as a function of the number of evidences. Results in the top two panels are associated with the event count summaries and in the bottom panels with the potency summaries. Left and right panels correspond to 200 and 500 evidences, respectively. The shaded area indicates the initial surrogate model building. The red dots indicate consecutive individual results associated with one execution of the forward evaluator. The blue lines track the minimum discrepancy obtained during the inference process. Note that the difference between absolute minimum discrepancy values between event count and potency summaries does not point to a better solution for the event count summary; it is governed by the scales of the original metrics.

σ_p : in Figure 13a the posterior still resembles the corresponding prior in Figure 8, whereas in Figure 13b it departs from the original prior distribution.

Figure 14 shows that the blue posterior means approach the red ground truth values. Reconstruction of the effective post-injection stresses in Figures 14b and 14d is much more accurate than reconstruction of the unsaturated pre-injection stresses in Figures 14a and 14c for both 200 and 500 evidences, and the posterior means also improve when increasing evidences from 200 to 500.

Comparing the two target functions highlights trade-offs in constraining the stress field. The event count target function improves with more evidences but is more sensitive to prior distributions, however with 500 evidences it quantifies a larger uncertainty zone, at substantially higher computational cost. For this target, the average deviation, computed as the mean-absolute-error of the estimated stresses from the ground truth is 29 and 23 MPa for 200 and 500 evidences, respectively.

In contrast, the total potency target function identifies optimal stress parameter values with fewer evidences and is more robust to prior assumptions, making it useful when prior knowledge is sparse or uncertain. The average deviation of the estimated stresses from the ground truth is 11 and 4 MPa for 200 and 500 evidences, respectively, corresponding to relative improvements of about 62% and 82% over the event count target for 200 and 500 evidences. Figure 15 shows that minimum discrepancy decreases during the BOLFI inversion; the upper and lower panels in Figure 15 correspond to event count and potency target functions, respectively. Using two independent realizations with different initial conditions, the minimum discrepancy converges to approximately 3 and 6 for event count and potency target functions, respectively, approaching the ground-truth minimum discrepancy values in Figures 9 and 12. Additionally, the event count-based posterior distributions, particularly for σ_p , depend more strongly on the prior than the potency-based results in Figure 10: the event count-based posterior for σ_p largely maintains the prior shape in Figure 8, leading to a higher posterior mean than the simulation ground truth.

Overall, target function selection and evidence count critically shape the precision and reliability of inferred ambient principal stress values. The total potency target function, with lower prior sensitivity and effective performance at moderate evidence counts, is the better choice for stress inversion in geothermal reservoirs as implemented here.

6. Discussion

The inversion results emphasize that the choice of the summary statistics is not a technical detail but a core modeling decision that controls the inversion of the ambient stress field. In this study, potency based summaries provide more informative constraints than event count summaries because they encode where deformation and energy release occur. Event counts can capture spatial occurrence rates but do not encode event size or deformation. This qualitative interpretation is consistent with the quantitative performance metrics reported in Section 5, including the average deviation of estimated stresses from the synthetic ground truth. This observation has a direct implication for monitoring and inversion design for geothermal reservoirs. Summary statistics should preferentially represent deformation- and damage-related observables that are mechanistically linked to permeability evolution and stress redistribution. Potency represents total slip area and average slip displacement during rupture (Equations 15 and 16) and therefore provides a compact proxy for the mechanical work done by the deforming reservoir.

A second implication is that the achievable resolution is bounded even with an efficient inference engine. Figure 6 shows that quasi-stochasticity introduced by the random initial damage distribution produces an intrinsic discrepancy floor, and Figures 9 and 12 indicate that BOLFI converges toward this floor. In practice, this suggests that uncertainty quantification should explicitly separate the irreducible simulator variability due to randomness from the uncertainty due to limited evidence counts and imperfectly informative summaries. The sensitivity analysis in Figure 7 further illustrates why likelihood-free inference is needed because the mapping from stresses to potency is highly nonlinear and non-monotonic, and multiple stress configurations can produce similar potency patterns. Rather than seeking one-to-one relationships between individual parameters and observables, the inversion should be framed as a probabilistic search for regions of parameter space consistent with the observed summaries. Beyond stress inversion, the workflow naturally generalizes to the inference of additional reservoir-relevant parameters. Permeability can be inferred by augmenting the target function with fluid flux measurements at the injection point and damage-state indicators linked to permeability such as microseismicity density or fracture density.

Finally, the value of BOLFI is strongest when forward models are expensive and likelihoods are intractable. Within the broader landscape of high-dimensional Bayesian and likelihood-free inversion such as sequential Monte Carlo methods, surrogate-assisted MCMC, and modern amortized neural SBI, BOLFI occupies a sample-efficient niche by explicitly steering simulator evaluations via Bayesian optimization. This approach can be coupled to more complex and computationally expensive THMC solvers to support hypothesis testing consistent with frameworks such as Wellmann et al. (2011). For high-dimensional problems where traditional direct-search approaches (Sambridge, 1999a, 1999b) become inefficient, the BOLFI-driven workflow provides an alternative path to quantify trade-offs and resolution using a limited number of forward evaluations.

7. Conclusion

This pilot study demonstrates a practical workflow for ambient-stress inversion in a quasi-stochastic EGS setting by coupling HydroPED with BOLFI. A key result is that target-function choice materially controls the quality and robustness of inferred stresses; in our synthetic test case, deformation-informed observables such as potency yield substantially smaller average deviations from the ground truth than occurrence-count summaries (Section 5). The scope of this study is intentionally limited: we use synthetic catalogs and a homogeneous model setup with initial damage seeding. Accordingly, the results should be interpreted as a proof of concept for sample-efficient likelihood-free inversion with an expensive forward model, rather than as a validated field-scale stress estimation method.

The main assumptions and limitations are that the stochastic initial damage distribution introduces an intrinsic discrepancy floor (Figure 6) that bounds attainable resolution, the quasi-static HydroPED simulator does not resolve dynamic rupture processes, and the inference is conditioned on the chosen priors, summary statistics, and discrepancy definition. These limitations also motivate future work. Future work should extend the inversion from stress-only to the estimation of other reservoir-relevant parameters such as permeability and injection or flux-related parameters by combining potency with additional observables, test alternative spatial summaries that better exploit source-mechanism information, and apply the workflow to field data with explicit treatment of observational uncertainty and model discrepancy. To reduce wall-clock time while retaining uncertainty quantification, an emulator can be tested in place of the full high-fidelity simulator HydroPED.

Appendix A: Mechanical Module

The mechanical module uses the EDFLM method to solve solid force equilibrium and fluid mass conservation (Cundall, 1988). This approach provides a significant advantage over conventional finite element methods for the cases of material instability. The module addresses the constitutive relation and the evolution of damage using Equations 2 and 6 in the main text, respectively (Shalev & Lyakhovsky, 2013). The damage-dependent poroelastic constitutive relationship involves stress and strain (Equation 2) and incorporates nonlinear elastic dilation during shearing (Hamiel, Lyakhovsky, & Agnon, 2004; Shalev & Lyakhovsky, 2013). The numerical implementation involves first solving a force balance equation for each node in the mesh described by

$$\frac{\partial V_i}{\partial t} = \frac{F_i}{m}, \quad (\text{A1})$$

where V_i is the velocity of a node of mass m when a force F_i is applied to the node. These nodal velocities are used to compute strain tensors and subsequently stress tensors (Levin et al., 2020; Shalev & Lyakhovsky, 2013). The method uses an adaptive time step described by

$$\Delta t = \frac{1}{2} \frac{\Delta x}{V_p}, \quad (\text{A2})$$

where Δx is the minimum distance between the nodes and V_p is the maximum possible seismic velocity in the material, which is a function of rock density and is subsequently decreased as the square root of a density scale factor (Shalev & Lyakhovsky, 2013). Damage levels are iteratively computed, and if critical damage is reached, stress drop and plastic strain accumulation occur, ensuring local solution without the need for a global stiffness matrix (Shalev & Lyakhovsky, 2013). The irreversible strain in the system is described by

$$\frac{de_{ij}^v}{dt} = \begin{cases} C_v \frac{d\alpha_D}{dt} \left(\sigma_{ij} - \frac{1}{3} \sigma_{kk} \delta_{ij} \right), & \frac{d\alpha_D}{dt} > 0 \\ 0, & \frac{d\alpha_D}{dt} < 0, \end{cases} \quad (\text{A3})$$

where e_{ij}^v is the irreversible strain, C_v is the irreversible strain parameter, σ_{ij} is the stress tensor, and σ_{kk} is the diagonal of the stress tensor. A more detailed description of the mechanical module is given by Shalev and Lyakhovsky (2013).

Appendix B: Fluid Flow Module

The fluid diffusion Equation 7 in the main text is solved using its weak form

$$(S + \Theta H \Delta t) p^{n+1} = L^T \Delta u + [S - (1 - \Theta) H \Delta t] p^n + F \Delta t, \quad (\text{B1})$$

where $0 \leq \Theta \leq 1$ is the time stepping weight coefficient and Δu is the incremental displacement. The S term is

$$S = \int_{\Omega} N^T S_e N d\Omega, \quad (\text{B2})$$

where N and N^T are the shape functions and their transpose vectors respectively. The H term is

$$H = \int_{\Omega} B^T k B d\Omega, \quad (\text{B3})$$

where B and B^T are gradients of the shape functions and their transpose vectors. The L^T term is

$$L^T = \int_{\Omega} N^T \alpha_B B d\Omega, \quad (B4)$$

and the F term is

$$F = - \int_{\Gamma} N^T q d\Gamma - \int_{\Omega} B^T k B \rho g \nabla z d\Omega, \quad (B5)$$

where q is the fluid source term (Shalev & Lyakhovsky, 2013). In these expressions, Ω and Γ represent the volume and the boundary of the computational domain, respectively. The linear algebraic equations are solved to obtain the pressure on each element (Shalev & Lyakhovsky, 2013). The consistency between the 3D grid and tetrahedral elements in the implementation of the Explicit Finite Difference Lagrangian Method eliminates the need for interpolation between modules (Shalev & Lyakhovsky, 2013). Hydrological changes are considered small, allowing the hydrological step to be performed after multiple solid deformation steps (Levin et al., 2020). Shape functions are recalculated at each time step, and permeability is subsequently updated (Shalev & Lyakhovsky, 2013). A third party parallel solver called the HSL solver is used to efficiently solve the large stiffness matrices and load vectors. A more detailed description of the fluid flow module is also given by Shalev and Lyakhovsky (2013).

Appendix C: Acquisition Rule

The unnormalized posterior distribution is calculated based on the predicted discrepancies obtained by computing the mean and variance of the surrogate model. In this study, the mean is set to zero and the maxvar acquisition rule is used to compute the variance of the surrogate model based on the available simulated observations. The maxvar acquisition rule evaluates the point where the current uncertainty in the unnormalized ABC posterior distribution is largest, ensuring that the algorithm samples regions where the improvement in accuracy of the estimation is needed most (Järvenpää et al., 2019). This is achieved by solving the optimization problem given by

$$\theta_{t+1} = \arg \max_{\theta} (p(\theta))^2 V(p_a(\theta)|D_{1:t}) \quad (C1)$$

where θ refers to the future parameter evaluation, $V(p_a(\theta)|D_{1:t})$ is the current variance of the un-normalized ABC posterior distribution, and Θ is the entire parameter space. See Equation 10 in Järvenpää et al. (2019) on how the variance is calculated. Järvenpää et al. (2019) also proposed a stochastic variant in which the next parameters are sampled from

$$\theta_{t+1} \sim p_q(\theta), \quad (C2)$$

where $p_q(\theta) \propto (p(\theta))^2 V(p_a(\theta)|D_{1:t})$ is the importance probability, $p(\theta)$ is the prior and $p_a(\theta)$ is the acceptance probability. The reader is encouraged to consult Järvenpää et al. (2019) and the corresponding supplementary material for details on the maxvar algorithm.

Appendix D: Algorithm

Algorithm 1 : BOLFI with maxvar acquisition

```

1: for  $t = 1, \dots, N_{\text{init}}$  do
2:   Generate  $\theta_t \sim p(\theta)$ 
3:   Generate  $y' \sim p(y|\theta_t)$ 
4:   Calculate  $d_t = d(s(y_{\text{obs}}), s(y'))$ 
5: end for
6: Set  $\varepsilon_{N_{\text{init}}} = \{(\theta_t, d_t)\}_{t=1}^{N_{\text{init}}}$ 
7: Fit  $d(\theta) | \varepsilon_{N_{\text{init}}} \sim GP(\mu_{N_{\text{init}}}(\theta), v_{N_{\text{init}}} + \sigma^2)$ 
8: for  $t = N_{\text{init}} + 1, \dots, N_{\varepsilon}$  do
9:   if  $t \equiv T_{\text{update}} \pmod{T_{\text{update}}}$  then
10:    Optimize GP hyperparameters
11:   end if
12:   Generate  $\theta_t \sim p_q(\theta)$  where  $p_q(\theta) \propto (p(\theta))^2 V(p_a | \varepsilon_{t-1})$ 
13:   Generate  $y' \sim p(y|\theta_t)$ 
14:   Calculate  $d_t = d(s(y_{\text{obs}}), s(y'))$ 
15:   Set  $\varepsilon_t = \varepsilon_{t-1} \cup \{(\theta_t, d_t)\}$ 
16:   Fit  $d(\theta) | \varepsilon_t \sim GP(\mu_t(\theta), v_t, \sigma^2)$  based on  $\varepsilon_t$ 
17: end for
18: Define  $L(\theta) \approx \Phi\left(\frac{h - \mu_t(\theta)}{\sqrt{v_t(\theta) + \sigma^2}}\right)$ , where  $h$  is the positive scalar bandwidth of the GP kernel.
19: Generate  $N_{\text{sample}}$  draws from approximate posterior distribution  $\propto L(\theta)p(\theta)$ 

```

Conflict of Interest

The authors declare no conflicts of interest relevant to this study.

Availability Statement

There are no seismic or other data used in this study. The stress estimates used to inform our synthetic examples are obtained from Kwiatek et al. (2019) and Kukkonen et al. (2023). All codes and notebooks used for the simulations and inference can be accessed publicly without restriction at Atobra (2025). BOLFI can be accessed at <https://elfi.readthedocs.io>.

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