

RESEARCH ARTICLE OPEN ACCESS

Probabilistic Identification of Parameters in Dynamic Fracture Propagation

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Received: 12 February 2025 | **Revised:** 1 January 2026 | **Accepted:** 22 January 2026

Keywords: Bayesian inference | dynamic fracture | embedded strong discontinuity | multiphase approach | uncertain input parameters

ABSTRACT

In this paper, we propose a novel multiphase approach for identifying input parameters in dynamic fracture propagation. Often, such parameters are partially known and uncertain with incomplete input data, resulting in challenges in predicting a reliable dynamic failure response. To address this, we employ a stochastic Bayesian inverse method to estimate input parameters in three distinct phases of a fracture model. As a case study, we analyze a virtual version of Kalthoff's dynamic fracture propagation test using a finite element model enhanced with embedded strong discontinuities, where cracks propagate in a mixed-mode manner, to demonstrate the effectiveness and robustness of the proposed method. The approach successfully identifies six material parameters, including the bulk modulus, shear modulus, tensile strength, shear strength, and the modes I and II fracture energies. Through different time intervals and measurements in each phase, our results show that the computed posterior mean values are closely aligned with the true parameters of the material, validating the reliability and accuracy of the method.

1 | Introduction

Reliable prediction of dynamic fracture propagation is important and challenging for researchers and engineers due to underlying complex, fast-evolving, destructive processes that are often difficult to observe directly in experiments. Numerical simulations play a crucial role in this task, as well as in understanding and improving material and structural performance in several scientific and engineering disciplines. Traditionally, various types of methods and models have been developed for simulations of the dynamic fracture propagation processes. Among these, the extended finite element method (X-FEM) introduces global discontinuous enrichment for cracks and the crack tip [1–4]. The embedded discontinuity finite element method alternatively incorporates strong discontinuities at the local element level and has been successfully applied in dynamic fracture propagation problems [5–8]. In contrast, phase field models use the smoothing approach over a crack region [9, 10]. Furthermore, discrete and lattice element models have been extensively addressed in dynamic failure propagation problems [11–14]. Although these methods are successful in representing dynamic fracture

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propagation problems, their responses depend heavily on the proper choice of input material and model parameters. Such parameters reflect material composition and heterogeneity, while guiding crack propagation mechanisms and dissipation.

Traditionally, certain material parameters can be determined through specially designed experimental setups that measure these parameters directly, such as in the case of re-enforced concrete, the yield stress of steel bars, or the bond shear stress [15]. However, more complex setups with multiple material parameters to be identified are challenging to implement in the laboratory setting, which is often the case for fracture propagation, where fracture energies can not be measured directly.

The fracture parameters can be calibrated using experimental analysis with the help of inverse methods, also known as model updating techniques [16]. While the *forward problem* describes the operator, that maps the fracture parameters to the structural behaviour (e.g., the displacement field)—given by some differential equations and solved by the above described FEM techniques, the *inverse problem* involves working backward from the observed outcomes of structural behaviour (e.g., relative displacements) to deduce the input fracture parameters that led to those observations. The classical approach to this calibration problem is through optimization, where a loss function is defined, which is to be minimized. This loss quantifies the discrepancy between simulation results and measurements. The problem of such an optimization problem is that it is typically ill-posed, for example, because multiple parameter values can yield the same loss, requiring ad-hoc regularization techniques; and even with those one may end up with some local minima. In contrast, Bayesian identification automatically renders the problem well-posed by inherently incorporating regularization through the integration of prior knowledge, while yielding a probability distribution instead of one deterministic value (cf. e.g., [17–19]). In this way, the Bayesian approach provides a comprehensive understanding of the uncertainty associated with the calibrated model coefficients. This information is crucial in the calibration process as it offers a nuanced perspective on the reliability and robustness of the calibrated model, setting Bayesian identification apart as a powerful and informative tool in the field of parameter estimation and model fitting in mechanics related problems, as shown in elastic [20, 21], nonlinear elastoplastic [22] and damage mechanics models [23]. Recent literature highlights the successful application of probabilistic approaches to fracture mechanics problems [24–29] as well as their effectiveness in accurately detecting failure surfaces and estimating failure of probabilities [30, 31]. However, to the authors' knowledge, no contributions have yet been made to the Bayesian identification of mechanical and material parameters in dynamic fracture propagation scenarios.

In both cases, either following the conventional optimization method, or the more advanced, probabilistic framework, the calibration process involves a huge number of evaluations of the deterministic forward solver with different values of its input fracture parameters. Unfortunately, even for small problems of fracture mechanics, especially when dealing with dynamic fracture problems, this evaluation requires significant computing power and time. One way to computationally ease this burden is to replace the computationally expensive high fidelity model by a so-called *surrogate model* (also known as *meta* or *proxy model*), which can turn the resource-intensive—if feasible at all—task at hand into a faster alternative, enabling a more efficient calibration processes. It is also true that the computation of an accurate surrogate model may also require a large number of forward solver calls. Nevertheless, while calibration methods often require a successive evaluation of the deterministic forward problem, computation of a surrogate model is amenable to parallelization and distributed computing, facilitating the exploration of parameter spaces concurrently. In addition, proxy models can provide insights into the sensitivity of the model parameters across a broader parameter space. Sensitivity analyses using surrogate models help to identify influential parameters and contribute to a better understanding of the model behavior, guiding the calibration process more effectively. There are several alternatives for surrogating such as Kriging, Fourier-expansion, deep neural networks, etc. Here, we will employ a *general Polynomial Chaos Expansion* (gPCE), using a linear combination of multivariate polynomials that are orthogonal with respect to the underlying probability measure defined by the prior description of the parameters. The gPCE as a surrogate model for Bayesian identification offers several advantages, especially in scenarios involving complex and high-dimensional systems [18, 19, 32, 33]. The gPCE is also well-suited to easily quantify uncertainties in the system, as well as to evaluate global sensitivities [34], using only the coefficients of the expansion.

Even for quasi-static problems, the derivation of a precise surrogate model for fracture mechanics poses a formidable challenge due to the inherently non-smooth nature of the response surface [28]. This intricacy arises prominently in temporal proximity to critical time steps associated with material state transitions, specifically transitions from an elastic state to a fractured state. Another challenge arises from the necessity to precisely characterize the model behaviour, which demands a high resolution in the displacement process. Achieving this precision mandates the incorporation of numerous time steps, contributing to a substantial increase in the dimensionality of the model output.

Taking the problem of bifurcation apart, one way to tackle the problem of non-smooth behaviour and the high-dimension of the output, is a parametric description of the model output in the time domain [27]. Such a representation of the output process is given by parameters (coefficients), which are assumed to depend smoothly on the model inputs. Unfortunately, such parametric representations have limitations, especially when dynamic fracture models are considered which produce highly complex model outputs.

This paper introduces several novel aspects to the field. Firstly, it departs from conventional optimization approaches, and, instead, employs probabilistic model updating, offering a more informative description of the parameters estimated. Secondly, the proposed probabilistic updating methods go beyond quasi-static analyses, covering dynamic fracture propagation driven by inertial forces and stress wave propagation within the embedded discontinuity finite element framework. This broader applicability enhances the versatility of the approach across a spectrum of fracture mechanics contexts. Thirdly, a distinctive feature lies in the adoption of a non-parametric methodology for the low-rank representation of measurable outputs based on the Proper Orthogonal Decomposition (POD). This approach removes limitations associated with parametric methods, thereby enhancing the flexibility and accuracy of the model. The paper also addresses a critical aspect by acknowledging and accommodating the increased inaccuracy of the surrogate model during pivotal time steps. This is achieved through the deliberate selection of a measurement error model that not only considers inherent errors due to the measurement device, but also effectively captures modeling discrepancies, thus contributing to a more comprehensive and realistic representation of the system dynamics. Lastly, another novelty of the paper is that it proposes a sequential update of the model parameters by dividing the identification process into three phases, based on sensitivity measures, namely into elastic, tensile fracture, and shear fracture phases. The identification in such a way is reduced to working in a very low-dimensional space of the parameters, requiring to update only a few parameters in each phase. The principles and results of the proposed approach can be equally applied to both two-dimensional or three-dimensional analyses. The demonstration example considers Kalthoff's test [35], an in-plane dynamic fracture propagation experiment in which a crack in a pre-cracked rectangular plate is impacted by a projectile and driven by inertial forces. In this case, the influence of the third dimension on crack propagation is negligible.

The flow of this paper is as follows. First, in Section 2, we give a short overview on the modelling of dynamic fracture propagation by an embedded discontinuity model, the computation of the forward problem, and introduce its abstract formulation. In Section 3 we show how to change this formulation to a stochastic setting, and describe the probabilistic model updating procedure using Bayesian updating by sampling from the posterior distribution of the fracture parameters using the *Markov Chain Monte Carlo* (MCMC) method. Secondly, we describe a gPCE of the low-rank representation of the measurable model output. To demonstrate the applicability of the presented procedure, we showcase it on the dynamic fracture model of the Kalthoff's test [35] in Section 4. Here, after presenting the deterministic model and deriving the low-dimensional representation of its measurable output, we describe the derivation of the surrogate model and the three-phase updating procedure. The paper closes with concluding remarks in Section 5.

2 | Embedded Discontinuity Model for Dynamic Fracture Propagation

To simulate complex fracture processes, a two-dimensional displacement-based solid finite element model, enriched with incompatible modes and an embedded strong discontinuity, is employed. This finite element, referred to as Q6ED, was introduced in [7]. This section provides a brief overview of the modelling procedure, including the cracking criteria and constitutive relations.

2.1 | Kinematic Relations

Consider a quadrilateral finite element e illustrated in Figure 1. A discontinuity line Γ^e divides the element area into Ω^{e+} and Ω^{e-} , such that $\Omega^e = \Omega^{e+} \cup \Gamma^e \cup \Omega^{e-}$ and $\Omega^{e+} \cap \Omega^{e-} = \emptyset$. Then, the displacement field $\mathbf{u} = [\mathbf{u}_x, \mathbf{u}_y]^T$ within the element, expressed in terms of nodal quantities, is given by

$$\mathbf{u}(\xi, \Gamma^e) = \sum_{a=1}^4 N_a(\xi) \mathbf{d}_a + \sum_{b=1}^2 M_b(\xi) \boldsymbol{\rho}_b + \sum_{i=1}^2 p_i(\xi, \Gamma^e) \alpha_i, \quad (1)$$

where $\mathbf{d}_a = [u_{xa}, u_{ya}]^T$ are the nodal displacements, $M_1(\xi) = 1 - \xi^2$ and $M_2(\eta) = 1 - \eta^2$ are the interpolation functions defined in the local coordinate frame (ξ, η) , associated with the incompatible modes $\boldsymbol{\rho}_b$. The interpolation functions

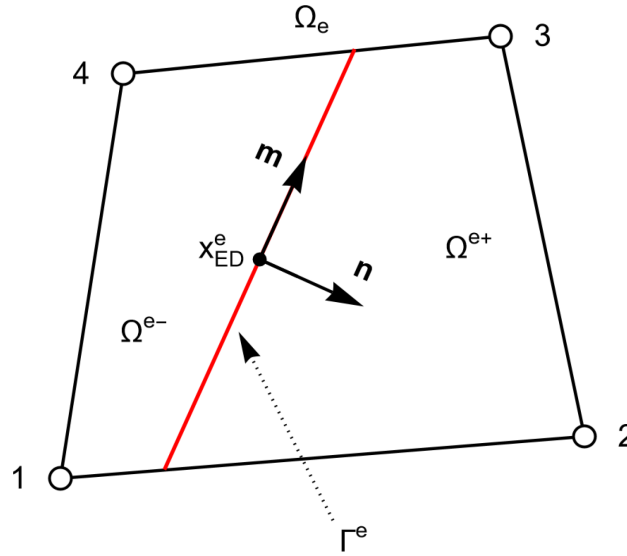


FIGURE 1 | Quadrilateral finite element Q6ED with discontinuity line Γ^e .

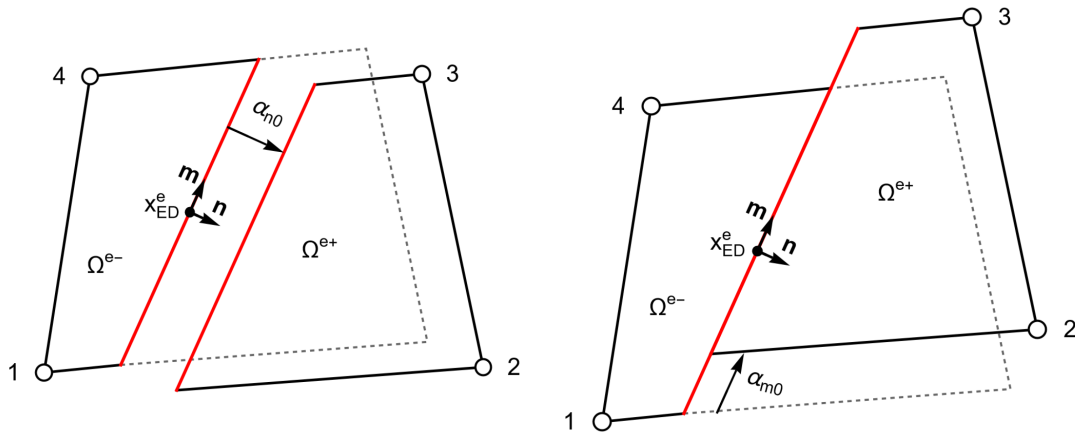


FIGURE 2 | Q6ED with separation modes at discontinuity line Γ^e ($\alpha_1 = \alpha_{n0}$, $\alpha_2 = \alpha_{m0}$).

$p_i = [p_{ix}, p_{iy}]^T$ correspond to the crack opening parameters α_i , illustrated in Figure 2. The second term in Equation (1) represents the contribution of the incompatible modes, which enhances the accuracy of the displacement field description under bending loading conditions. This improvement in displacement field accuracy leads to a more precise stress field, which is critical for the crack nucleation criteria. When a crack is activated, the third term in Equation (1) introduces the jump-in-displacements at the embedded discontinuity line, represented as a linear combination of two opening parameters α_i , where i denotes the direction of the opening. The jump-in-displacements are interpolated over the finite element using the interpolation functions

$$p_1 = \left(H_\Gamma(\mathbf{x}) - \sum_{a \in \Omega^{e+}} N_a \right) \mathbf{n}, \quad p_2 = \left(H_\Gamma(\mathbf{x}) - \sum_{a \in \Omega^{e+}} N_a \right) \mathbf{m}. \quad (2)$$

Here, $\mathbf{n} = [n_x, n_y]^T$ and $\mathbf{m} = [m_x, m_y]^T = [-n_y, n_x]^T$ are the unit normal and unit tangent to Γ^e , respectively. H_Γ is the Heaviside function, which is equal to unity for $\mathbf{x} \in \Omega^{e+}$ and vanishes otherwise. This function introduces a strong discontinuity in the displacements along Γ^e . The strain field is obtained by applying the symmetric gradient operator to Equation (1). Further details on this procedure and the model development can be found in [7].

2.2 | Constitutive Relations

Before the initiation of the fracture process, the solid body exhibits elastic behavior, which is modelled using the linear Hooke's law. Once a crack nucleates, it may open in Mode I and/or Mode II manner. The behaviour along the discontinuity

line is described using two independent rigid-damage constitutive laws. For mode I opening, the corresponding Helmholtz free energy is expressed by

$$\Psi_n(\bar{u}_n, \bar{Q}_n, \bar{\xi}_n) = \frac{1}{2} \bar{Q}_n^{-1} \bar{u}_n^2 + \bar{\Xi}(\bar{\xi}_n), \quad (3)$$

where $\bar{Q}_n$ is the compliance modulus for Mode I, $\bar{u}_n$ represents opening normal to the discontinuity line, and $\bar{\Xi}(\bar{\xi}_n)$ is a softening potential dependent on internal softening variable $\bar{\xi}_n$.

The failure function for softening, which enforces the unilaterality of Mode I failure (allowing only $\bar{u}_n \geq 0$), is defined as

$$\bar{\phi}_n(t_n, \bar{q}_n) = t_n - (\sigma_{un} - \bar{q}_n) \leq 0, \quad (4)$$

where σ_{un} denotes the tensile strength, and $\bar{q}_n$ represents the softening traction (thermodynamic force) associated with $\bar{\xi}_n$ given by

$$\bar{q}_n = \frac{\partial \bar{\Psi}_n}{\partial \bar{\xi}_n} = \sigma_{un} \left(1 - \exp \left[-\frac{\sigma_{un}}{G_{fn}} \bar{\xi}_n \right] \right), \quad (5)$$

with G_{fn} being the Mode I fracture energy. Similarly, in tangential direction to the embedded discontinuity line (Mode II), the failure function is defined as

$$\bar{\phi}_m(t_m, \bar{q}_m) = |t_m| - (\sigma_{us} - \bar{q}_m) \leq 0, \quad (6)$$

where σ_{us} is the shear strength, and $\bar{q}_m$ is the softening traction in the tangential direction. The model permits sliding along the discontinuity line in both directions. For more details please refer to [7].

2.3 | Crack Initiation

To ensure that the fracture model reflects the physical behavior of the material, each crack line needs to be embedded at the right instance, the right place, and oriented in the proper direction. This process is governed by the crack initiation criterion presented in [7, 36]. For each intact finite element, the principal stresses

$$\sigma_{p1,p2}^{e,i} = \frac{\sigma_{xx}^{e,i} + \sigma_{yy}^{e,i}}{2} \pm \sqrt{\left(\frac{\sigma_{xx}^{e,i} - \sigma_{yy}^{e,i}}{2} \right)^2 + (\sigma_{xy}^{e,i})^2} \quad (7)$$

at each i th integration point are computed to evaluate the onset of cracking. Then, the maximum first principal stress

$$\sigma_p^{e,i} = \max(\sigma_{p1}^{e,i}, \sigma_{p2}^{e,i}), \quad i = 1, \dots, 4 \quad (8)$$

is written out for each integration point. When at least one principal stress exceeds the material tensile strength, that is, $\sigma_p^{e,i} \geq \sigma_{un}$, the procedure for determining the position and orientation of embedded discontinuity line within the finite element begins. The set

$$B^e = \{id \in \{1, 2, 3, 4\} : \sigma_{p1}^{e,id} = \sigma_p^e\} \quad (9)$$

contains the indices of integration points where the material strength σ_{un} is exceeded. The discontinuity line goes through the centroid of the integration points collected in the set B^e , and its position is given by

$$\mathbf{x}_{ED}^e = \frac{1}{N_{B^e}} \sum_{i \in B^e} \mathbf{x}^{e,i}, \quad (10)$$

where N_{B^e} is the total number of elements in B^e and $\mathbf{x}^{e,i}$ is the position vector of the i -th integration point in the global coordinate system. The direction of the embedded discontinuity depends on the average stress

$$\sigma_{ED}^e = \frac{1}{N_{B^e}} \sum_{i \in B^e} \sigma^{e,i} \quad (11)$$

in the integration points from B^e . Here, we take the components of the average stress σ_{ED}^e to determine the angle of the discontinuity line α_{ED}^e

$$\alpha_{ED}^e = \frac{1}{2} \arctan\left(\frac{2\sigma_{xyED}^e}{\sigma_{xxED}^e - \sigma_{yyED}^e}\right), \quad (12)$$

which aligns with the direction of the normal vector $\mathbf{n}$ orthogonal to the crack. No crack tracking algorithm is needed, and new crack lines may appear within multiple finite elements in a single time step. For more details, the reader is referred to [7].

2.4 | Equilibrium Equations

From the principle of virtual work one obtains three different stationary equations. The first equilibrium equation is

$$\mathbf{R}_d^e = \mathbf{f}^{ine,e} + \mathbf{f}^{int,e} - \mathbf{f}^{ext,e} = \mathbf{0}, \quad (13)$$

where $\mathbf{f}^{ine,e}$ is the vector of element inertial forces, $\mathbf{f}^{int,e}$ is the vector of internal forces in the element and $\mathbf{f}^{ext,e}$ is the vector of external forces on the element. The inertial force vector, $\mathbf{f}^{ine,e}$, depends on the material's mass density $\bar{\rho}$ and the acceleration. The acceleration is computed using Newmark's standard implicit integration scheme with the trapezoidal rule ($\gamma = 1/2, \beta = 1/4$).

The second stationary equation is a local equation at the element level, given by

$$\mathbf{R}_\alpha^e = \mathbf{0}, \quad (14)$$

which enforces the equivalence between the resultant force due to tractions along the discontinuity line Γ^e , and the resultant force arising from stresses in the bulk. Solving Equation (14) yields the values of crack opening parameters α_i (see Equation (1)). The third equilibrium equation is also a local condition at the element level, and is expressed as

$$\mathbf{R}_\rho^e = \mathbf{0}, \quad (15)$$

which is related to the incompatible modes and returns the values of incompatible parameters ρ_b (see Equation (1)).

The governing Equations (13–15) form an augmented system of equations, which is subsequently reduced to include only the nodal displacements $\mathbf{d}_a$ by eliminating α_i and ρ_b . The resulting condensed system is then sent to the assembly procedure to construct the global system of equations for the entire finite element model. Solving the global system yields the unknown degrees of freedom in the vector $\mathbf{d}_a$, which are used to compute the corresponding local element values of α_i and ρ_b . For additional details on the solution procedure readers are referred to [7].

3 | Probabilistic Identification

An overview of the probabilistic identification workflow is provided in the schematic flowchart shown in Figure 3. Let $\mathbf{q} \in \mathbb{R}^n$ represent a vector of the uncertain elastic and fracture input parameters of the embedded discontinuity finite element model (EDFEM). We model these parameters as random variables (RVs) denoted by $\mathbf{Q} : \Omega \rightarrow \mathbb{R}^n$ — Ω being the set of all possible outcomes—due to our lack of knowledge of their exact values. The uncertainty regarding the “true” values of the selected parameters is captured by the probability distribution $\pi_{\mathbf{Q}}(\mathbf{q})$ of these random variables.² This probability distribution $\pi_{\mathbf{Q}}(\mathbf{q})$ of the random vector $\mathbf{Q}$, which is also called the “prior” distribution, is intended to reflect the present engineering knowledge (based on e.g., experiments, professional expertise, and standards) on the potential parameter values and their associated probabilities.

Let us introduce the forward solution operator $\mathcal{S} : \mathbb{R}^n \rightarrow \mathbb{R}^m$ in an abstract form. This operator maps the uncertain parameters $\mathbf{q}$ to a global vector $\mathbf{u}_g$ comprising all nodal displacements $\mathbf{d}_a$ for each FEM node, incompatible modes ρ_b , and the crack opening parameters α_i for each element, and all of these parameters are registered for each simulated pseudo-time step. As discussed in Section 2, the operator $\mathcal{S}$ cannot be expressed explicitly, but is instead computed through a complex, sequential numerical procedure.

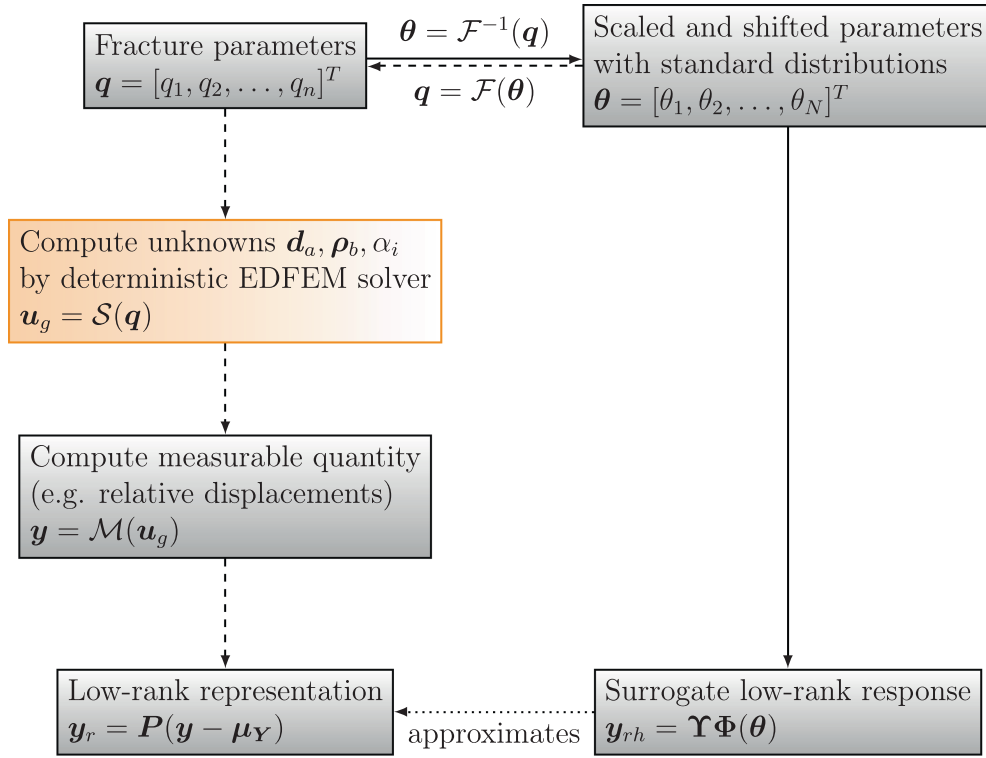


FIGURE 3 | Replacing the deterministic EDFEM solver by a gPCE surrogate model: the dashed line shows the path without a surrogate model and the continuous line shows the one when a surrogate model is used.

Furthermore, let us assume some measurable quantity, $\mathbf{y} \in \mathbb{R}^L$, which is computed by some *measurable operator* $\mathbf{y} = \mathcal{M}(\mathbf{u}_g)$. Such a measurable quantity can for example be the relative displacement between two points of the test for different time steps. The actual measurements measured on a test with material properties $\mathbf{q}_m$ will then take the form

$$\mathbf{z}_m = \mathcal{M} \left(\underbrace{S(\mathbf{q}_m)}_{\mathbf{u}_g} \right) + \epsilon, \quad (16)$$

where ϵ is one realization of the vector of random variables $\mathbf{E} : \Omega \rightarrow \mathbb{R}^L$ representing the sum of the modelling error and the measurement noise. We denote the probability density of the error model $\mathbf{E}$ by π_E .

3.1 | Bayesian Inference-Parameter Update

Following the probabilistic framework for the parameters identification, what is needed is the distribution of the parameters conditioned on the specific measured value $\mathbf{z}_m$ of the measurable quantity $\mathbf{y}$, termed the “posterior” distribution. This distribution is expressed by Bayes’s theorem

$$\underbrace{\pi_{Q|\mathbf{z}_m}(\mathbf{q})}_{\text{posterior}} = \frac{\overbrace{\pi_{\mathbf{z}_m|Q}(\mathbf{q})}^{\text{likelihood}} \overbrace{\pi_Q(\mathbf{q})}^{\text{prior}}}{\underbrace{\int_{I_Q} \pi_{\mathbf{z}_m|Q}(\mathbf{q}) \pi_Q(\mathbf{q}) d\mathbf{q}}_{\text{evidence}}} = \frac{\mathcal{L}(\mathbf{q}) \pi_Q(\mathbf{q})}{\zeta}, \quad (17)$$

where the numerator is the product of the likelihood and the prior, and the denominator, also called the evidence, is just the normalization factor assuring that the density function integrates to one. The likelihood $\mathcal{L}(\mathbf{q}) = \pi_{\mathbf{z}_m|Q}(\mathbf{q})$ of measuring a specific value of the measurable quantity $\mathbf{z}_m$ given a certain value of the parameter $\mathbf{q}$ can be computed by determining the probability of the measurement error taking value $\epsilon = \mathbf{z}_m - \mathbf{y}$, that is,

$$\mathcal{L}(\mathbf{q}) = \pi_E(\mathbf{z}_m - \mathcal{M}(S(\mathbf{q}))). \quad (18)$$

The Bayesian posterior distribution can be computed using the random walk of the Metropolis-Hastings algorithm, a Markov Chain Monte Carlo (MCMC) sampling procedure, which iteratively generates samples from the posterior based on the likelihood and prior distributions. This approach enables efficient exploration of the parameter space, yielding robust posterior estimates even for complex models. Unfortunately, such a procedure is computationally intensive as it requires evaluating the likelihood at each step of the random walk. Consequently, every iteration demands a deterministic EDFEM solver call to evaluate $\mathcal{M}(S(\mathbf{q}))$, leading to an exceedingly high computational cost when the number of iterations is large. Furthermore, the procedure can get highly unstable when the dimension of the measurable output is high, producing extremely small values for the likelihood. This may also be the case, when the MCMC procedure is based on the log-likelihood instead of the likelihood. To master these challenges, we first introduce a low-rank representation of the measurable quantity and a surrogate model to replace the computationally expensive EDFEM solver.

3.2 | Low-Rank Representation of the Measurable Output

In the example of the dynamic fracture problem considered here, the dimension m of the measurable quantity $\mathbf{y}$ (as well as the measurement $\mathbf{z}_m$ itself) is relatively high. This is due to the fact that many measurement locations and many measured time steps are needed for the calibration process of the dynamic fracture problem. To reduce the dimension of the measurable input, a low-rank representation is proposed, which is computed by projecting the measurable quantity with a projection matrix $\mathbf{P}$. To get an optimal projection matrix, where the loss of information is as small as possible, one may use the proper orthogonal decomposition (POD) of the measurable vector. For that, let us first decompose the measurable vector into its mean value and its fluctuating part, which is to be further decomposed by the POD,

$$\mathbf{Y}(\omega) = \boldsymbol{\mu}_Y + \tilde{\mathbf{Y}}(\omega) = \boldsymbol{\mu}_Y + \mathbf{V}\mathbf{S}\mathbf{W}(\omega) = \boldsymbol{\mu}_Y + \sum_i \sigma_i \mathbf{v}_i W_i(\omega), \quad (19)$$

where ω represents the actual realization, that is the randomness of the vector, $\mathbf{S}$ is a diagonal matrix with $[\mathbf{S}]_{ii} = \sigma_i$, $\mathbf{V}$ an orthogonal matrix, and $\mathbf{W}(\omega)$ a vector of uncorrelated random variables, that is, $\mathbb{E}[W_i(\omega)W_j(\omega)] = \delta_{ij}$. The orthogonal matrix $\mathbf{V}$ can be computed from the eigenvalue decomposition of the covariance matrix of $\mathbf{Y}$, namely

$$\mathbf{C}_Z = \mathbb{E}[\tilde{\mathbf{Y}}\tilde{\mathbf{Y}}^T] = \mathbf{V}\mathbf{S}\mathbb{E}[\mathbf{W}(\omega)^T\mathbf{W}(\omega)]\mathbf{S}\mathbf{V}^T = \mathbf{V}\mathbf{S}^2\mathbf{V}^T = \sum_i \sigma_i^2 \mathbf{v}_i \mathbf{v}_i^T. \quad (20)$$

The POD then can be computed by solving the eigenvector problem

$$\mathbf{C}_Y = \mathbf{V}\mathbf{S}^2\mathbf{V}^T \quad (21)$$

$$\mathbf{C}_Y \mathbf{V} = \mathbf{V}\mathbf{S}^2 \quad (22)$$

$$\mathbf{C}_Y \mathbf{v}_i = \sigma_i^2 \mathbf{v}_i = \lambda_i \mathbf{v}_i. \quad (23)$$

For dimension reduction, the reduced representation $\mathbf{Y}_r$ of the measurable quantity $\mathbf{Y}$ is obtained by projecting its fluctuating part onto the space spanned by the $\mathbf{v}_i$ vectors. But instead of using all m eigenvectors, only a reduced number m_r is chosen which captures a given ratio of the total variance of the measurable vector $\mathbf{Z}$, expressed by

$$\rho_L = \frac{\sum_{i=1}^{m_r} \lambda_i}{\sum_{j=1}^m \lambda_j}. \quad (24)$$

The projection is given by

$$\mathbf{Y}_r = \underbrace{\mathbf{V}_r^T}_{\mathbf{P}} (\mathbf{Y} - \boldsymbol{\mu}_Y), \quad (25)$$

where $\mathbf{V}_r$ is the reduced matrix containing the first m_r eigenvectors $\mathbf{v}_i$.³

To perform the MCMC random walk using this reduced representation (which is often preferable), the measured values and the error model have also to be projected onto the reduced space. The projected measured value is computed as $\mathbf{z}_{rm} = \mathbf{P}(\mathbf{z}_m - \boldsymbol{\mu}_Y)$.

For example, if the measurement error consists of unbiased Gaussian random variables with a diagonal covariance matrix C_E —which is often the case—the projected error model will also be Gaussian. The new covariance matrix for the error is given by $C_{E_r} = PC_E P^T$. The posterior distribution is then expressed using the same form as in Equation (17), but replacing z_m with z_{mr} and computing the modified likelihood $\mathcal{L}_r$ using the projected error distribution

$$\mathcal{L}_r(q) = \pi_{E_r}(z_{mr} - P(\mathcal{M}(S(q)) - \mu_Y)). \quad (26)$$

3.3 | Surrogate Modelling

For the complex system describing dynamic fracture, directly simulating the measurable output $\mathcal{M}(S(q))$ from the uncertain parameters at each random step of the MCMC computation is computationally prohibitive. To mitigate this, we construct a surrogate model using Generalized Polynomial Chaos (GPC) expansion, which offers an efficient and accurate approximation of Y or rather its projected version Y_r (see figure 7). In the GPC framework, Y_r is approximated as a finite series expansion of orthogonal polynomial basis functions $\Phi_i(\theta)$,

$$y_r(q(\theta)) \approx y_{rh}(q(\theta)) = \sum_{i=0}^P v_i \Phi_i(\theta) = Y\Phi(\theta), \quad (27)$$

where v_i are the GPC coefficients, $\Psi_i(\theta)$ are multivariate polynomials orthogonal with respect to the probability density function of the so called *germs* θ , and P is the total number of terms retained in the expansion. Here, the vector of independent variables θ with standard distributions is introduced for computational convenience, to be transformed to the uncertain random variables q . This transformation is defined by the mapping

$$q = F(\theta). \quad (28)$$

In our example, we suppose that the elements of q are independent, and θ is derived by shifting and scaling the components of the vector q to standardize their distribution.

The choice of the polynomial basis depends on the distribution of the uncertain parameters; for example, Hermite polynomials are used for Gaussian distributions, while Legendre polynomials are used for uniform distributions. The gPC coefficients v_i can be computed by regression using input-output pairs q_i and $y(q_i)$ computed by the EDFEM.⁴

The gPC coefficients v_i in the expansion (27) can be computed using several established methods [32]. One common approach is the *orthogonal projection* (or pseudo-spectral projection, which exploits the orthogonality of the polynomial basis $\Phi_i(\theta)$ with respect to the probability measure of θ to directly project the model outputs onto the polynomial basis using some quadrature rules (e.g., Gauss quadrature or Monte Carlo integration). Alternatively, the coefficients can be obtained via *regression-based methods*, where the coefficients are determined by fitting the model outputs at a finite set of realizations of θ . Sparse regression techniques, such as *least angle regression* (LAR), may be particularly effective when the required surrogate complexity is high, for example, when a large polynomial degree is needed. These methods enable the identification of a reduced subset of basis functions from the full polynomial basis (constructed up to a prescribed maximal degree), retaining only the most relevant terms in the expansion [37, 38]. Other approaches employ truncated basis based on hyperbolic index sets or more advanced incremental techniques based on this truncated basis and on LAR [37]. Alternatively, a posteriori filtering strategies first compute the full basis and then retain only those terms whose contribution to the output variance exceeds a prescribed threshold [39]. All of these non-intrusive methods are widely used in the literature and provide flexible and efficient means for constructing accurate polynomial chaos surrogates.

4 | Numerical Example

This study focuses on identifying the unknown material parameters governing dynamic fracture. In our research, two software packages are employed. AceFEM [40], a finite element environment integrated within Wolfram Mathematica [41], is used to implement the two-dimensional finite element model and to perform numerical simulations of Kalthoff's test. Additionally, MATLAB 2024 [42] is utilized for the stochastic identification procedures. The following sections introduce Kalthoff's test, and explain the three phases of the stochastic identification procedure. The test is performed virtually in the computer, where the material parameters of this "truth" are known. The identification procedure can thus be tested in how well it is able to recover these values. Finally, the results from each phase are summarized and compared with the true values.

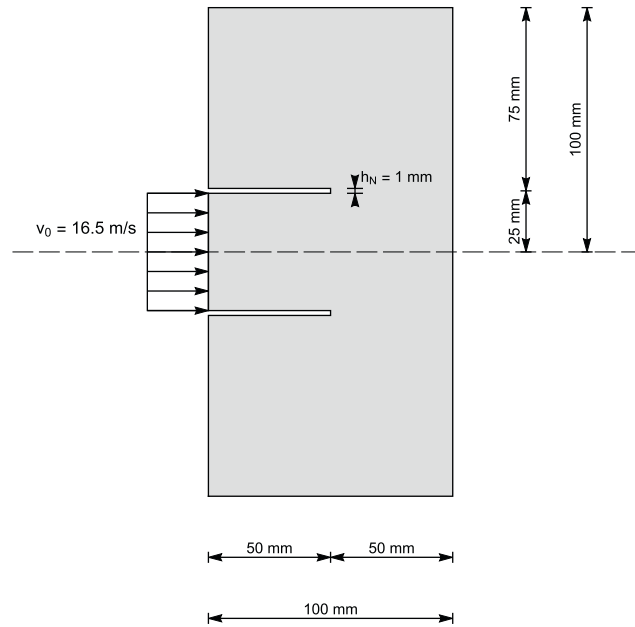


FIGURE 4 | Kalthoff's test: Geometry and boundary conditions.

4.1 | Kalthoff's Test

As an example of dynamic fracture, the experiment from [13, 14, 35], known as Kalthoff's test, is considered. A thin high-strength steel plate of thickness $t^e = 9$ mm, with two parallel notches (see Figure 4), is exposed to lateral impact load by a projectile that was launched from a gun muzzle with a velocity of 33 m/s. The experimental results showed that from each notch a tensile crack propagated at an angle of about 70° with respect to the notch line.

When preparing the numerical model, the virtual “truth,” we took into account the assumption from [43], saying that the specimen and the projectile have the same elastic impedance, and thereby the impact load of the projectile can be modelled by an imposed constant velocity of $v_0 = 16.5$ m/s—which is one-half of the projectile's velocity. The imposed velocity v_0 , which is applied on the edge between the two notches for 100μ s, is the only boundary condition in the finite element model. The material of the plate has mass density of $\bar{\rho} = 8000\text{kg/m}^3$.

4.2 | Modelling and Measurements

To build a numerical model of the whole thin plate for the virtual test, we use the quadrilateral finite element Q6ED from [7], formulated with plane stress assumptions. The Q6ED element is enhanced with incompatible modes for a better description of deformation in the bending case. The crack is represented by an embedded discontinuity line (see model and simulation results in Figure 5) as explained in Section 2.

To test the identification procedure, we assume that we lack the complete set of data required to perform the numerical simulation. To determine the unknown input parameters, we employ the stochastic Bayesian inverse method (see Section 3). A successful simulation of crack propagation requires six material parameters to be known,

$$\mathbf{q} = \left[K \ G \ \sigma_{un} \ \sigma_{us} \ G_{fn} \ G_{fs} \right]^T, \quad (29)$$

where K and G represent the bulk and shear moduli, σ_{un} and σ_{us} are the normal and shear strengths, and G_{fn} and G_{fs} are the fracture energies for Mode I and Mode II, respectively. Small uncertainties in these parameters propagate into large uncertainties in the measurable quantities $\mathbf{Y}$ of the dynamic fracture test, producing a complex response surface for $\mathcal{M}(\mathbf{S}(\mathbf{q}))$. This surface is difficult to simulate using the EDFEM, and thus we try to approximate it using a surrogate model. To address this, we adopt a multi-phase calibration approach, which separates the distinct effects of the uncertain parameters through tailored testing scenarios. By analyzing the entire virtual experiment, we observed that it can be divided

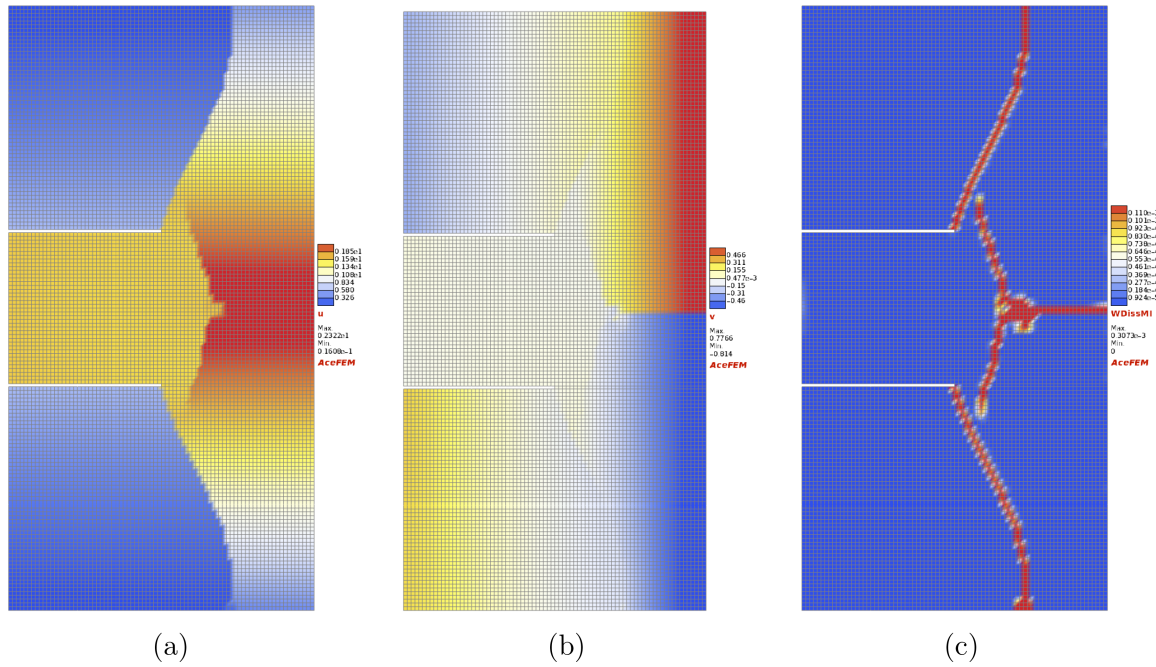


FIGURE 5 | Kalthoff's test: State of the model at the end of simulation. (a) Horizontal displacement u . (b) Vertical displacement v . (c) Dissipated fracture energy due to crack opening in Mode I manner.

TABLE 1 | Multi-phase identification of material parameters and the considered measurements.

Phase i	Dominant Behaviour	The parameters to be identified (q_i)	Start t_{is} [μs]	End t_{ie} [μs]	Measurements y_i [mm]
1	Elastic phase	K and G	0	20	u_{xj}, u_{yj} for $j = 1, \dots, 6$
2	Fracture in Mode I	σ_{un} and G_{fn}	0	50	ΔL_1 and ΔL_2
3	Fracture in Mode II	σ_{us} and G_{fs}	40	80	ΔL_3 and ΔL_4

into three significant phases, each governed by deformation behaviour that depends on only two material parameters. These three phases and the corresponding measurements are presented in Table 1 and Figure 6.

- **Phase 1: Elastic Properties (q_1)**

In the first phase, we focus solely on the elastic material properties by considering the uncertain parameter set $q_1 = [K \ G]^T$. The prior log-normal distributions for the unknown parameters are set to be

$$K \sim \log N(162.5, 40)[\text{GPa}] \quad \text{and} \quad G \sim \log N(75, 8)[\text{GPa}],$$

which was set based on best engineering judgment.

The dynamic test begins at the time instance $t_{1s} = 0 \mu s$ when the impact load strikes the plate (see Figure 4), and lasts until $t_{1e} = 20 \mu s$. The stress field remains within the elastic regime, which allows us to isolate and identify the values of K and G . The considered measurements are horizontal and vertical displacements u_x and u_y , a vector collecting the displacements at the different time steps in six nodal points located in the area between two notches as shown in Figure 6a and Table 2.

By measuring the horizontal displacements, we measure the velocity of seismic waves. It depends on the dynamic Young's modulus, density and Poisson's ratio. For a homogeneous material such as high strength steel the dynamic and static Young's moduli are very close which enables us the estimation of the static Young's modulus from the Kalthoff's test. In a similar manner we use the vertical displacements as a measurements of the seismic shear waves velocity to estimate the static shear modulus.

- **Phase 2: Mode I Fracture Parameters (q_2)**

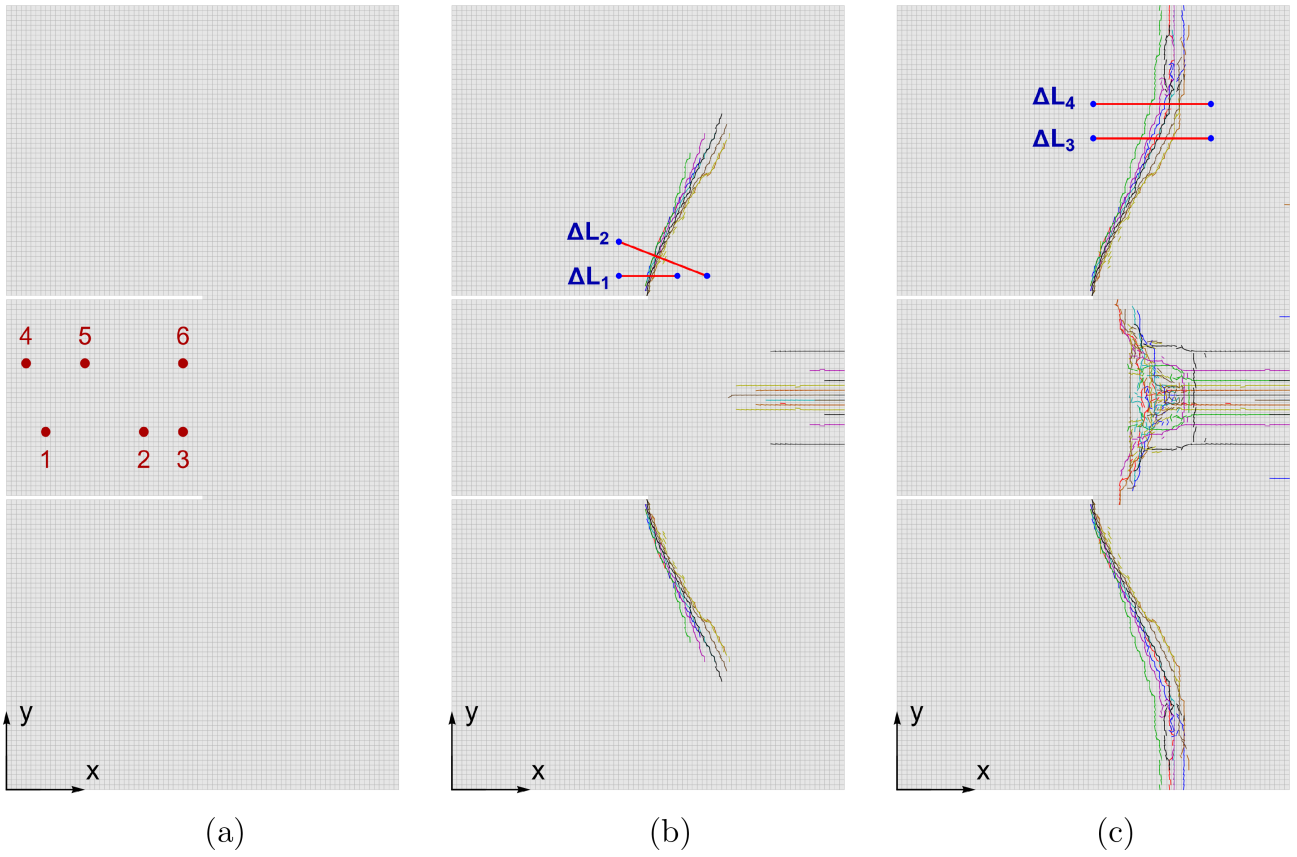


FIGURE 6 | Measurements in each phase of the identification. (a) Phase 1, (b) Phase 2, (c) Phase 3.

TABLE 2 | Phase 1: Location of observed points.

Point <i>i</i>	<i>x</i> [mm]	<i>y</i> [mm]	Measurement [mm]
1	10	91.25	u_x and u_y
2	35	91.25	
3	45	91.25	
4	5	108.75	
5	20	108.75	
6	45	108.75	

The second phase targets the Mode I fracture parameters, $\mathbf{q}_2 = [\sigma_{un} \ G_{fn}]^T$. The corresponding prior distributions are set to be the log-normal distributions

$$\sigma_{un} \sim \log N(0.750, 0.120) \text{ [GPa]} \quad \text{and} \quad G_{fn} \sim \log N(26.00, 5.00) \text{ [Nmm}^2\text{/mm]}.$$

A test is designed based on sensitivity analysis, ensuring that the measurable outputs vary solely due to changes in these two parameters. Several measurement configurations were evaluated, including nodal displacements and strain measurements taken at points located on one side of the crack path only. The sensitivity analysis revealed that σ_{un} and G_{fn} exhibit the greatest sensitivity to longitudinal deformations measured along lines intersecting the crack path. The onset of displacement discontinuity occurs when $\sigma > \sigma_{un}$, while the fracture energy G_{fn} is progressively dissipated as the crack propagates.

This approach enables precise calibration of σ_{un} and G_{fn} . It involves crack formation and Mode I crack opening. This phase spans the first 50 μs , that is, the time interval $[t_{2s}, t_{2e}] = [0, 50] \mu\text{s}$. During this phase, the deformation of two line segments ($\Delta\mathbf{L}_1$ and $\Delta\mathbf{L}_2$, see Figure 6b) is measured. These lines (or strain gauges) span over the possible crack

TABLE 3 | Phase 2: Location of observed points.

Point <i>i</i>	x_1 [mm]	y_1 [mm]	x_2 [mm]	y_2 [mm]	Measurement [mm]
1	42.50	31.02	57.5	31.02	ΔL_1
2	42.50	39.80	65	31.02	ΔL_2

TABLE 4 | Phase 3: Location of observed points.

Point <i>i</i>	x_1 [mm]	y_1 [mm]	x_2 [mm]	y_2 [mm]	Measurement [mm]
1	50	66.14	80	66.14	ΔL_3
2	50	74.92	80	74.92	ΔL_4

paths that begin at the end of the top notch, so that the crack initiation and corresponding jumps in displacements can be measured. The start and end points of these lines are provided in Table 3.

• Phase 3: Mode II Fracture Parameters (q_3)

In the third phase, the parameters identified in the previous steps are fixed to their expected values, and the focus shifts to the Mode II fracture parameters, $q_3 = [\sigma_{us} \ G_{fs}]^T$. The corresponding prior distributions are set to the log-normal distributions

$$\sigma_{us} \sim \log N(0.580, 0.100) \text{ [GPa]} \quad \text{and} \quad G_{fs} \sim \log N(26.00, 5.00) \text{ [Nmm}^2/\text{mm]}.$$

Similarly to Phase 2, various measurement configurations were analyzed through a sensitivity study in Phase 3. The results showed that the shear parameters σ_{us} and G_{fs} exhibit the highest sensitivity to the longitudinal deformation along the lines that intersect the crack path in the region of crack kinking. This corresponds to the so-called shear phase, characterized by mixed-mode (Mode I and Mode II) crack propagation that results in a kinking crack path. This phase occurs over the time interval from $t_{3s} = 40\mu s$ to $t_{3e} = 80\mu s$.

To identify the shear parameters, the considered deformations ΔL_3 and ΔL_4 are positioned in the vicinity of crack kinking, where the cracks open in a Mode II manner actively. The positions of ΔL_3 and ΔL_4 are given in Figure 6c and Table 4.

By systematically separating the effects of different parameter groups, this multi-phase approach ensures a more accurate calibration and reduces the complexity associated with the coupling of uncertain parameters. The multiphase approach is graphically represented in Figure 7. The following subsections, show the details, and the results of the Bayesian inference in each phase are provided.

4.3 | Phase 1: Identification of Elastic Parameters

To identify the elastic material parameters $q_1 = [K, G]$, we observe the local deformation in the first $20\mu s$ divided into 200 time steps. Our measurements are nodal displacements ($y_1 = [u_x, u_y]$) in six nodes distributed over the solid part in between the two notches, see Figure 6 and Table 2.

For the computation of the proxy or surrogate model, the FEM simulations are performed for a total of 5199 samples generated from different values of the input parameter vector q_i . The dataset includes 199 Gauss quadrature points (ranging from 2×2 to 7×7 tensor-product rules), which were initially generated to explore an orthogonal projection based polynomial chaos construction. However, due to the highly nonlinear and non-smooth response induced by the dynamic fracture behavior, this approach proved insufficiently accurate.

The surrogate model was therefore constructed using a regression-based approach. To adequately capture the complexity of the response surface, besides the already available quadrature point, the number of training samples was successively increased using quasi-Monte Carlo sampling based on a Halton sequence, resulting in a total of 5000 QMC samples. The

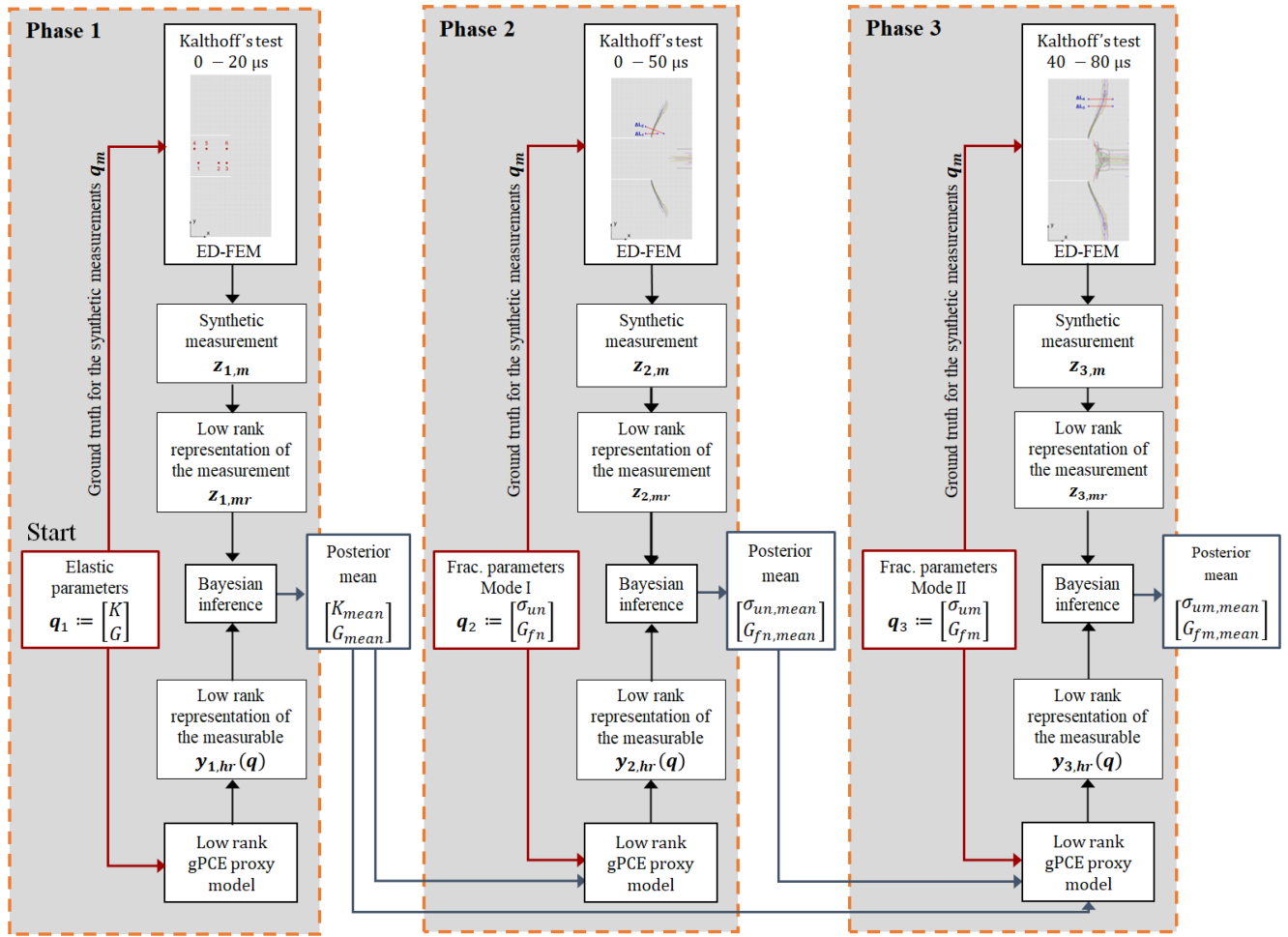


FIGURE 7 | Flowchart: Identification of parameters through three phases.

complete dataset was split into two groups: 4159 samples (80%) are used to train the model, while 1040 samples (20%) are reserved for testing the accuracy.

Sparse polynomial chaos techniques, including least angle regression (LARS) and variance-based truncation of polynomial terms, were also investigated. While these methods are effective for smoother problems, in the present dynamic fracture setting we observed that discarding terms with small individual variance contributions could nevertheless lead to a significant loss of global accuracy. Consequently, retaining the full polynomial basis was beneficial to ensure reliable surrogate predictions.

Despite the relatively large training set, the surrogate construction remains computationally feasible due to extensive parallelization of the deterministic solver. Moreover, the surrogate enables efficient MCMC sampling, which would otherwise require orders of magnitude more high-fidelity model evaluations.

The proxy model predicts the low-rank representation of the nodal displacements u_x and u_y in six assimilation points, as illustrated in Figures 6 and 8.

4.3.1 | Low-Rank Representation and Its Surrogate Model

After the impact, pressure and shear waves propagate through the elastic solid domain. The wave velocities depend on the stiffness of the solid. Consequently, different values of stiffness parameters $[K, G]$ lead to variations in wave propagation velocities causing them to reach the observed nodes at different time instances. This effect is illustrated in Figure 8, where different $[K, G]$ values result in distinct deformations at the observed nodes, occurring at varying time points. The latter introduces additional complexity for constructing a reliable proxy model. To address this, the measurements are projected onto a low-rank basis defined by the eigenvectors of the covariance matrix C_{Y_1} . This matrix is computed from the set of

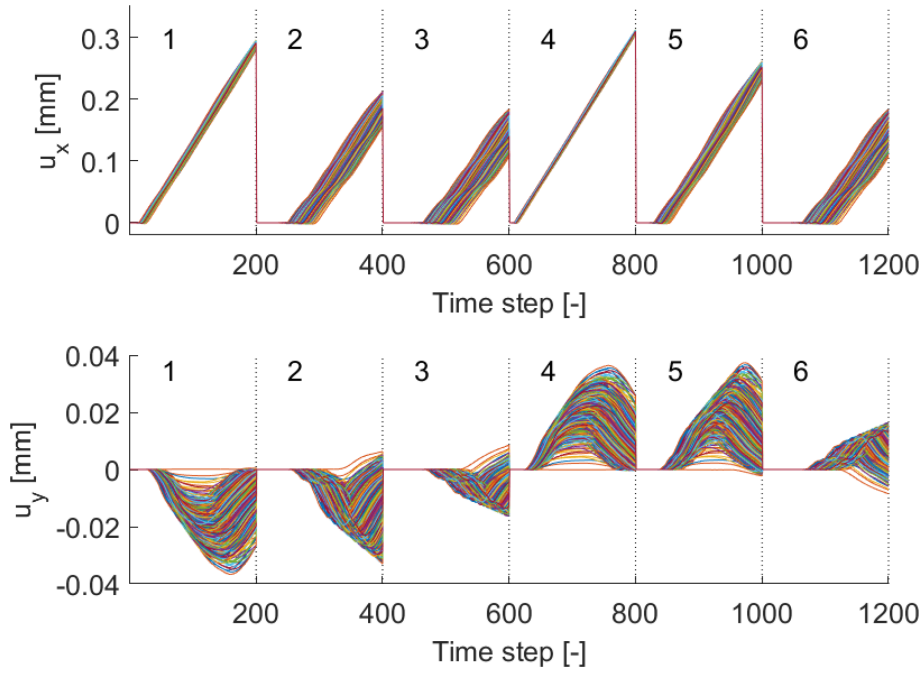


FIGURE 8 | Phase 1 – training samples used for building proxy models for u_x and u_y .

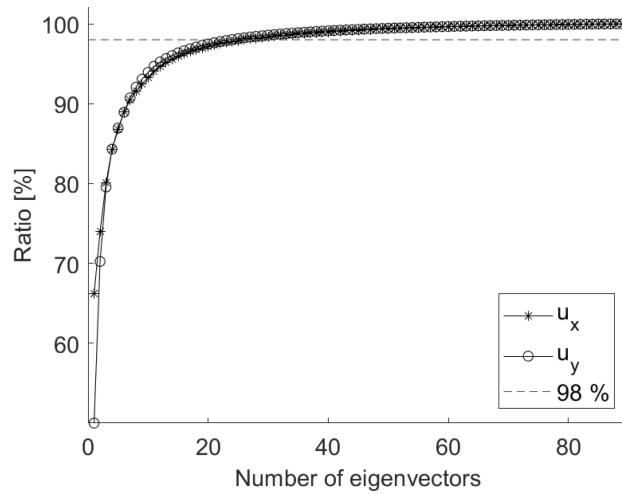


FIGURE 9 | Phase 1 – eigendecomposition of the covariance matrix for u_x and u_y .

training samples used for building the proxy model.⁵ The eigen-decomposition of the covariance matrix C_{Y_1} reveals that 30 eigenvectors are sufficient to capture 98% of the variation of Y_1 , see Figure 9.

Figure 10a illustrates how the mean absolute error (MAE) of the low-rank representation decreases for higher dimensions of the low-rank basis. At a dimensionality of 30, the MAE for the low-rank representation of the horizontal displacement u_x is 1.00e-05 mm, and for the vertical displacement u_y is 0.57e-05 mm.

Figure 10b summarizes the validation of the proxy model for different degrees of gPCE, evaluated using the testing samples. For the proxy model, we have selected a gPCE representation with a degree of 15. At this degree, the MAE for the horizontal displacement u_x is 1.88e-05 mm and for the vertical displacement u_y is 1.16e-05 mm.

4.3.2 | Statistics and Sensitivity

Figure 11 presented the results of the sensitivity analysis efficiently computed from the gPE coefficients [34]. As shown in the figure, the total variation in all displacements is predominantly attributed to the combined effect of variation in

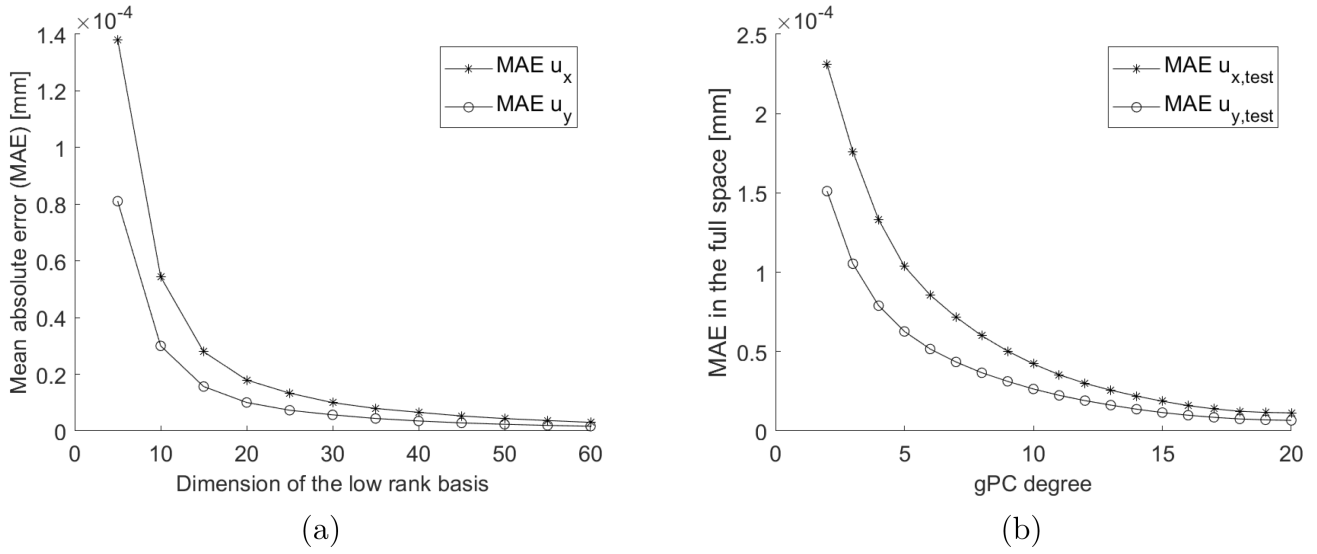


FIGURE 10 | Phase 1 – (a) Mean absolute error for different dimension of low-rank space for u_x and u_y (b) Mean absolute error for different degrees of gPCE for u_x and u_y .

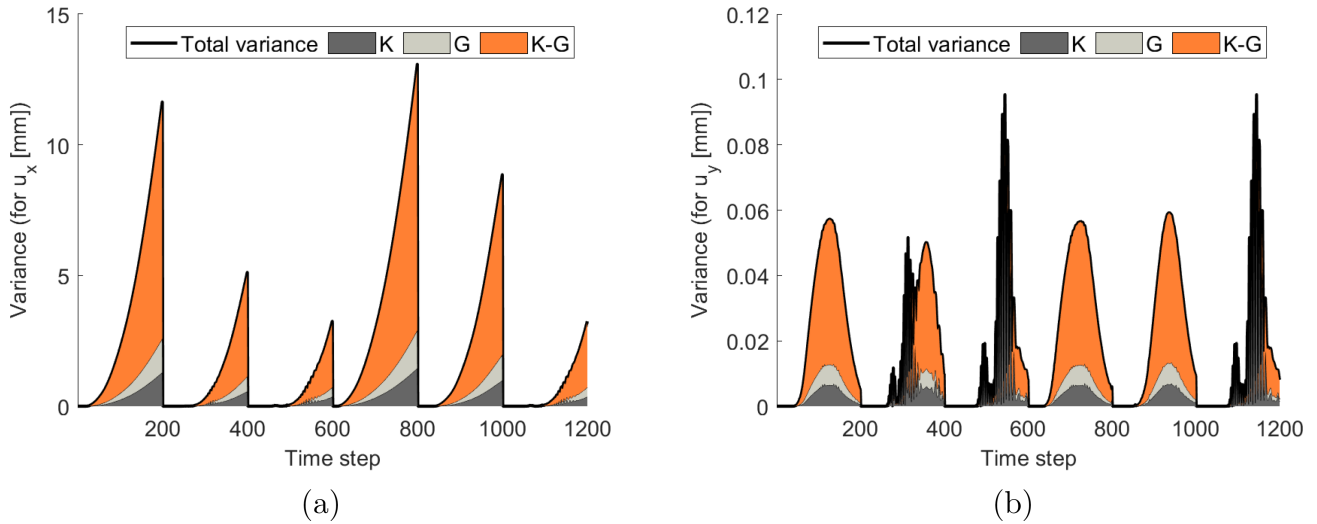


FIGURE 11 | Phase 1 – sensitivities of measurable variable Y_1 expressed by Sobol partial variances of (a) $u_{x,1}$ and (b) $u_{y,1}$ computed from the gPCE model.

the two elastic parameters, with smaller contributions arising from their individual, first-order effects. The diagram in Figure 11b for the vertical displacement u_y , shows noisy curves for points 2, 3, and 6. This noise is caused by the use of higher-order polynomials in the gPC proxy model with a degree of 15. Reducing the degree to 12 or lower would diminish the noise, but result in an unacceptably lower accuracy for the proxy model.

4.3.3 | Bayesian Updating by the Metropolis-Hastings Algorithm

To identify the unknown moduli K and G , we use the Bayesian update method described in Section 3. The error model E (see Equation (16)) is assumed to follow a normal distribution with zero mean and a diagonal covariance matrix C_{E_1} . The variances of C_{E_1} are computed from the standard deviation

$$\sigma_{E_1} = 0.002 \text{ mm} + \sigma_{\text{proxy},1}. \quad (30)$$

Here, $\sigma_{\text{proxy},1}$ represents the standard deviation of the modeling error which is due to the surrogating. This standard deviation is estimated from the testing data samples, by computing the discrepancy between surrogate model y_{h1} — mapped

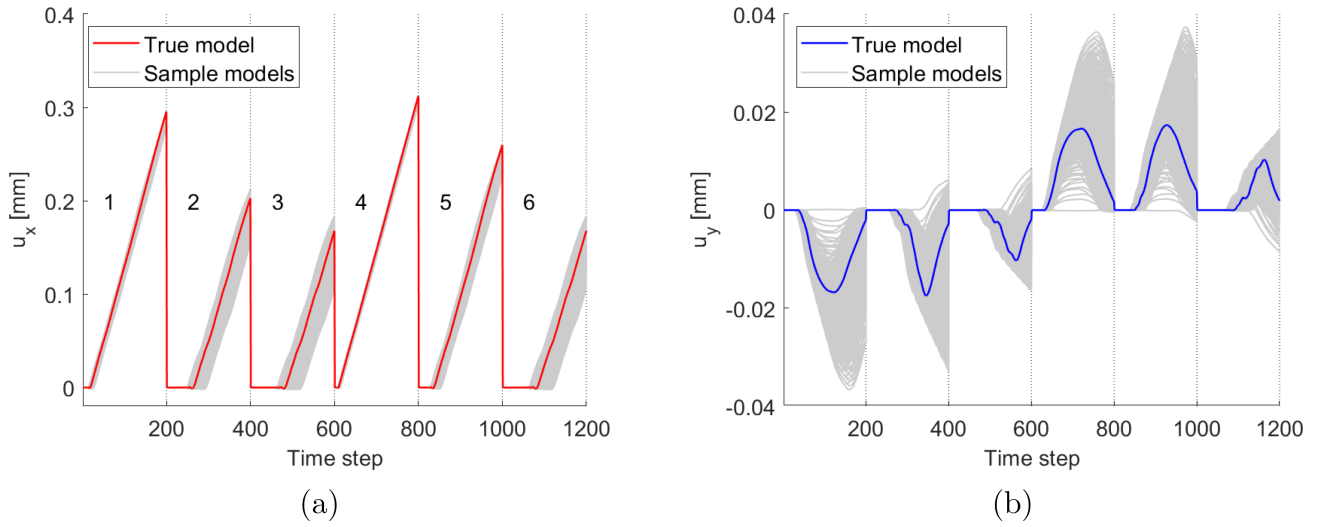


FIGURE 12 | Phase 1—Measurable variables computed from the ground truth and from a set of samples of the a-priori parameter distribution, (a) horizontal displacements $[u_x]$ and (b) vertical displacements $[u_y]$.

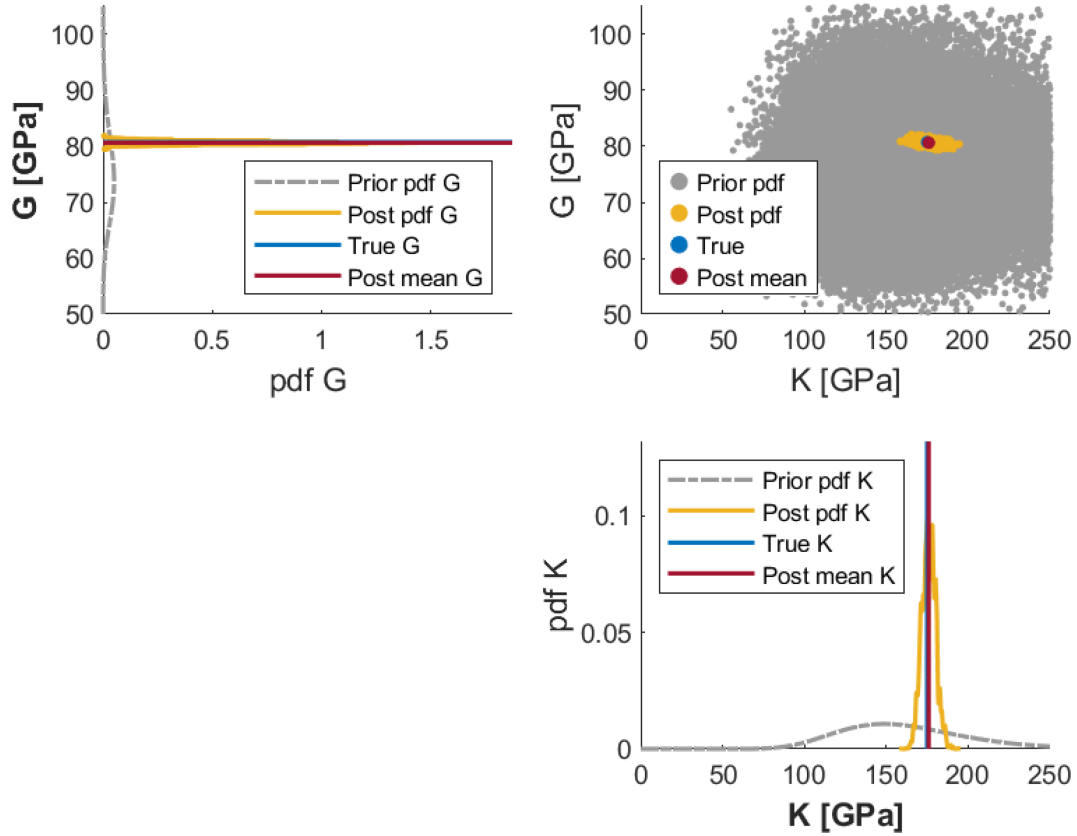


FIGURE 13 | Phase 1—A-priori distribution of the q_1 parameters and the samples of their a-posteriori distribution, as well as the mean of the posterior samples.

to the original, high dimensional space—and the original data computed by the EDFEM model. The synthetic or virtual measurement was generated by presuming a certain ground truth for the input parameter $q_{1,m} = [K_m, G_m]$ and adding to the simulated measurable response $y_{1,m} = \mathcal{M}(S(q_{1,m}))$ a sample from the measurement error model E_1 . As shown in Figure 12, the measurable variables computed from the true value $q_{1,m}$ lie within the range among the measurable variables obtained from the training samples.

Figure 13 presents the results of the Bayesian update in Phase 1. The resulting posterior mean for the bulk modulus K is 175.97 GPa with a standard deviation of 4.22 GPa, while the resulting posterior for the shear modulus G is 80.65 GPa with

a standard deviation of 0.33 GPa. The posterior mean values are used as deterministic value of the bulk and shear moduli in the following phases, that is, Phase 2 and 3.

4.4 | Phase 2: Tensile Strength and Fracture Energy for Mode I

In the second phase of the identification procedure, the tensile strength σ_{un} and the fracture energy G_{fn} are determined and incorporated into the q_2 vector of uncertain parameters. For this purpose, deformations $y_2 = [\Delta L_1, \Delta L_2]^T$ are observed as illustrated in Figure 6b. The analysis considers a time interval from 0 μs to 50 μs divided into 500 time steps. Figure 14 depicts 4052 samples (out of total 5065 samples) used for building the proxy model. These samples are projected into the low-rank space formed by 30 eigenvectors which capture 98% of the variance in the covariance matrix (computed from the training set samples). The low-rank representation is then substituted with the proxy model represented by the gPCE with total polynomial degree of 12.

Figure 15 presents the sensitivity analysis of the proxy model in the full rank space. The selected measurable quantities are sensitive to both parameters. The figure suggests that the relative displacements are less sensitive to the individual variations of the two parameters, while their joint variation has a more significant impact.

The error model E (see Equation (16)) for Phase 2 is similar to the one defined for Phase 1, that is described in Section 4.3.3. The variances of the covariance matrix C_{E_2} are computed from the standard deviation

$$\sigma_{E_2} = 0.004 \text{ mm} + \sigma_{\text{proxy},2}, \quad (31)$$

where $\sigma_{\text{proxy},2}$ is the standard deviation of the modeling error introduced by the proxy model.

Figure 16 summarizes the results of the Bayesian update procedure for the tensile strength σ_{un} and fracture energy G_{fn} . From the resulting joint posterior distribution the mean value of tensile strength σ_{un} is 0.84543 GPa with a standard deviation of 0.0259 GPa. For the fracture energy G_{fn} , the mean value is 22.13 Nmm²/mm with a standard deviation of 0.2156 Nmm²/mm. The posterior mean values of σ_{un} and G_{fn} are used as deterministic inputs in Phase 3.

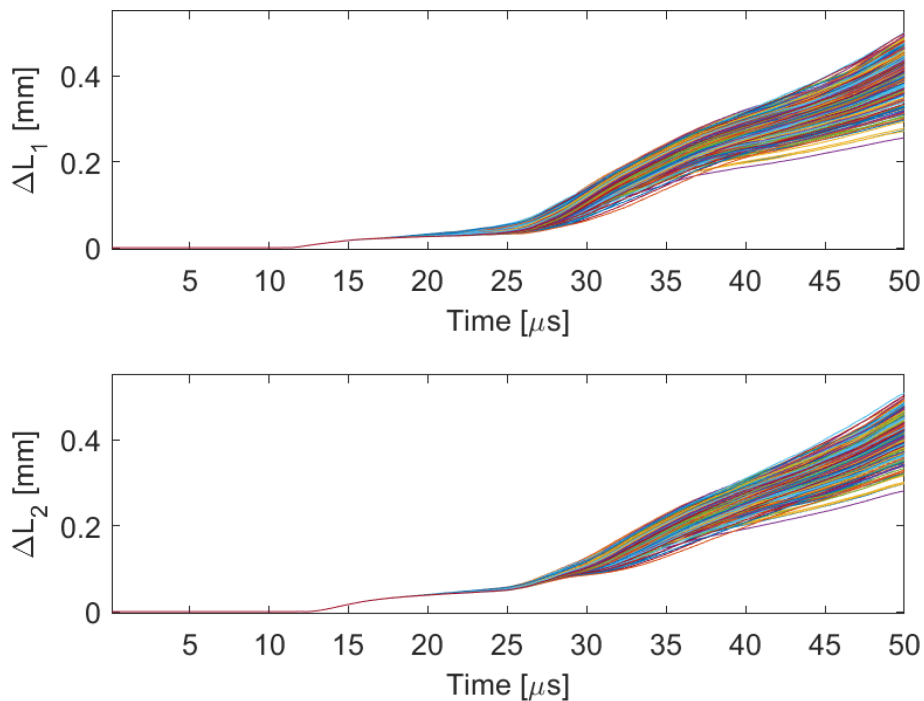


FIGURE 14 | Phase 2—Training samples used for building proxy models for ΔL_1 and ΔL_2 .

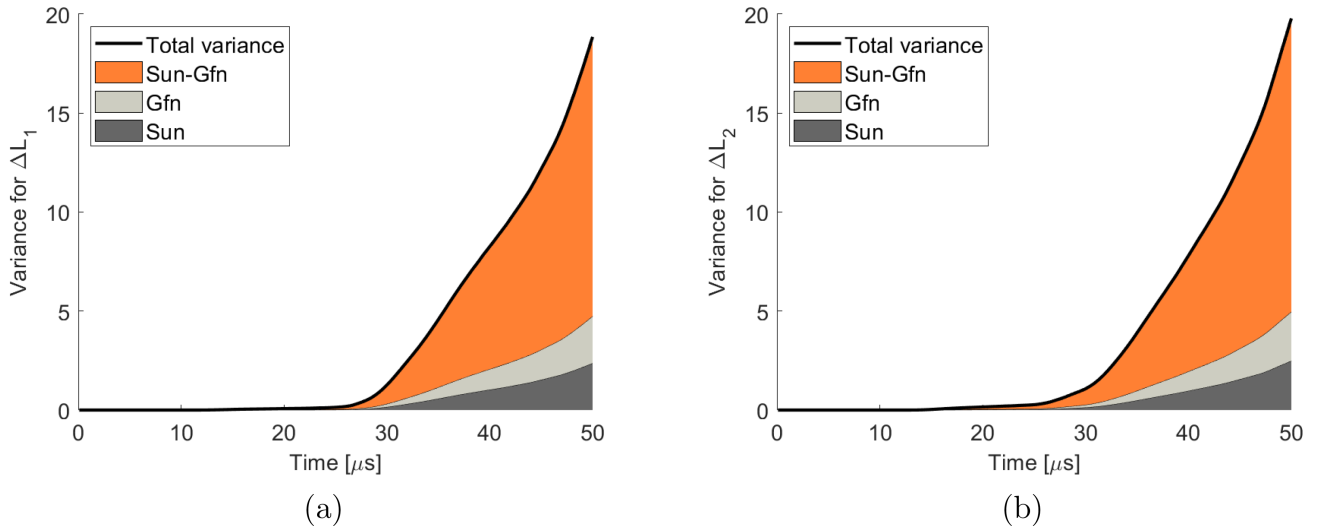


FIGURE 15 | Phase 2—sensitivities of measurable variable Y_2 expressed by Sobol partial variances of (a) ΔL_1 and (b) ΔL_2 computed from the gPCE model.

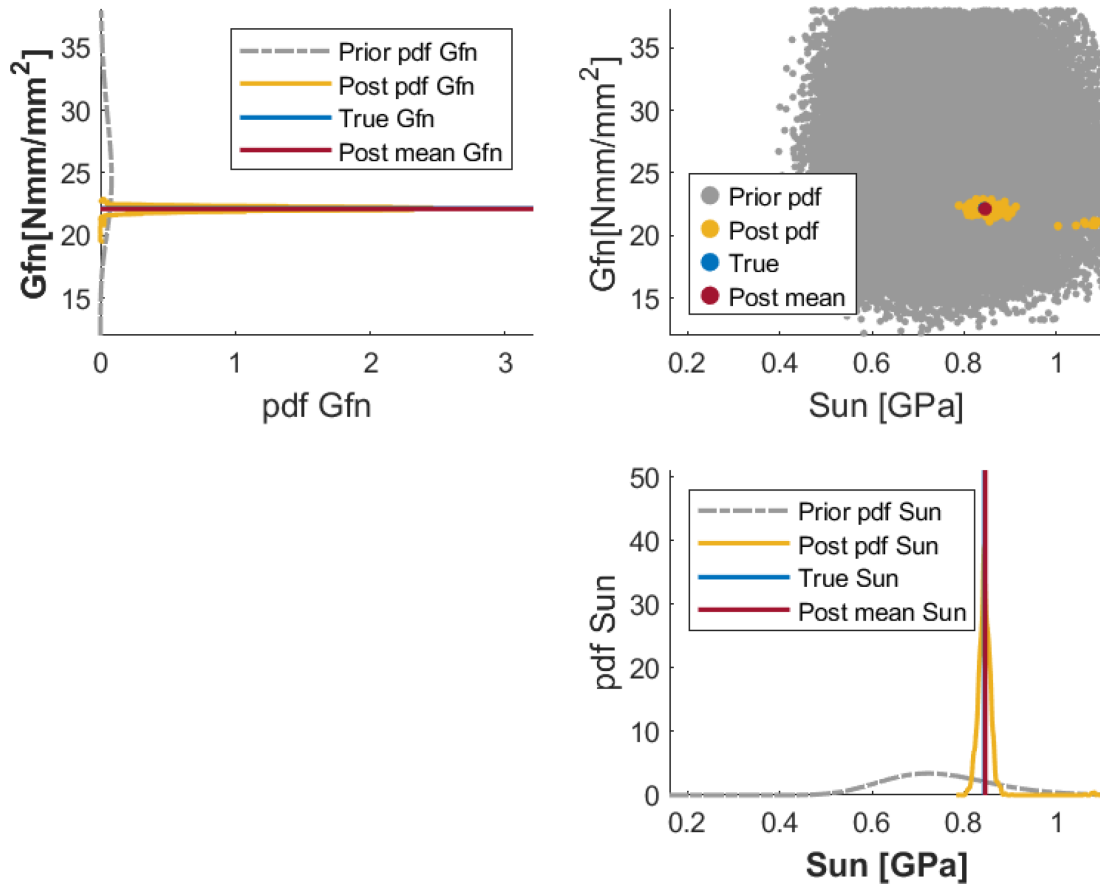


FIGURE 16 | Phase 2 – A-priori distribution of the v_{q_2} parameters and the samples of their a-posteriori distribution, as well as the mean of the posterior samples.

4.5 | Phase 3: Shear-Strength and Fracture Energy for Mode II

To identify the values of the uncertain parameters of the third phase q_3 , the shear strength σ_{us} and fracture energy for Mode II, G_{um} , the deformations $y_3 = [\Delta L_3, \Delta L_4]$ (see Figure 6c) are measured over time interval from 40 μs to 80 μs , divided into 401 time steps. This interval corresponds to the period during which cracks actively open in mode II.

Figure 17 shows 3919 samples (out of a total of 4909) used to construct the proxy model. The low-rank basis is defined by 40 eigenvectors, which capture 98% of the variance in the sample covariance matrix. The response of the proxy model is then projected back onto the full-rank basis for evaluation across different degrees of gPCE. Based on the validation of the gPCE proxy model, a polynomial degree of 10 was selected (Figure 18).

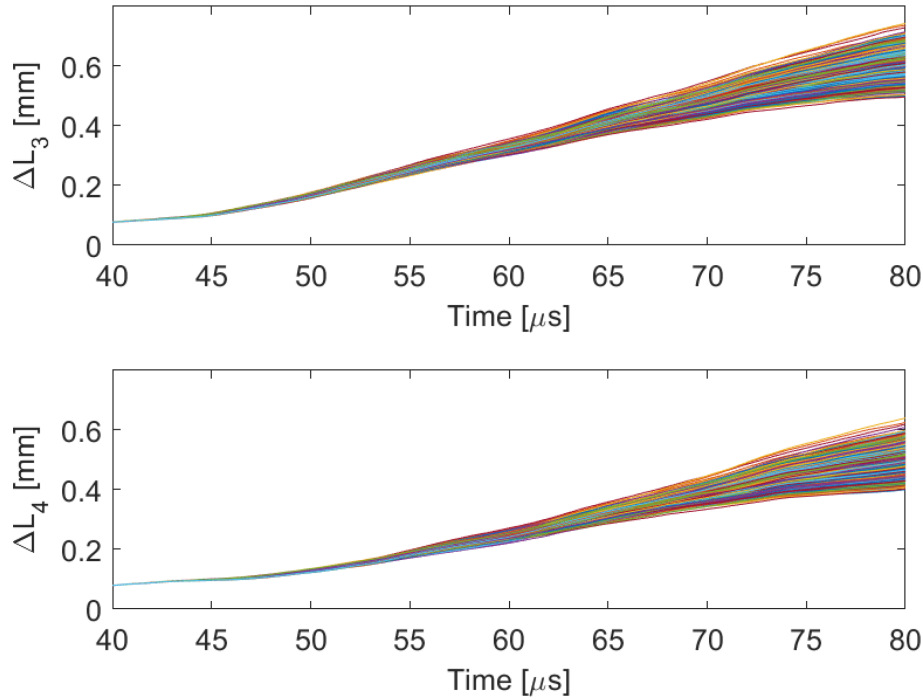


FIGURE 17 | Phase 3 – training samples used for building proxy models for δL_3 and δL_4 .

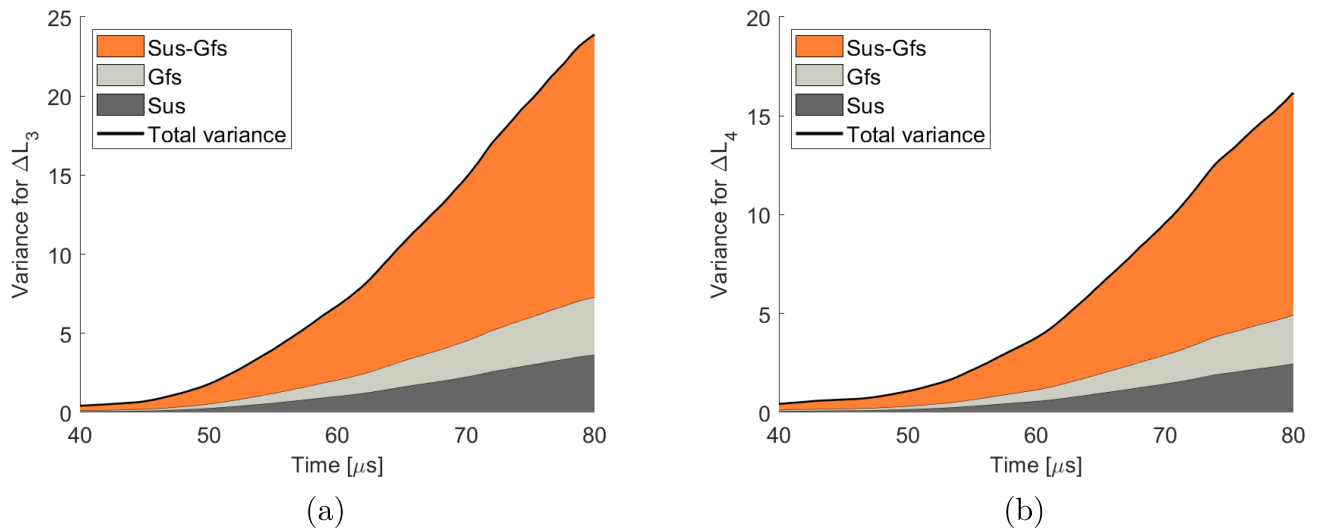


FIGURE 18 | Phase 3 – sensitivities of measurable variable Y_3 expressed by Sobol partial variances of (a) ΔL_3 and (b) ΔL_4 computed from the gPCE model.

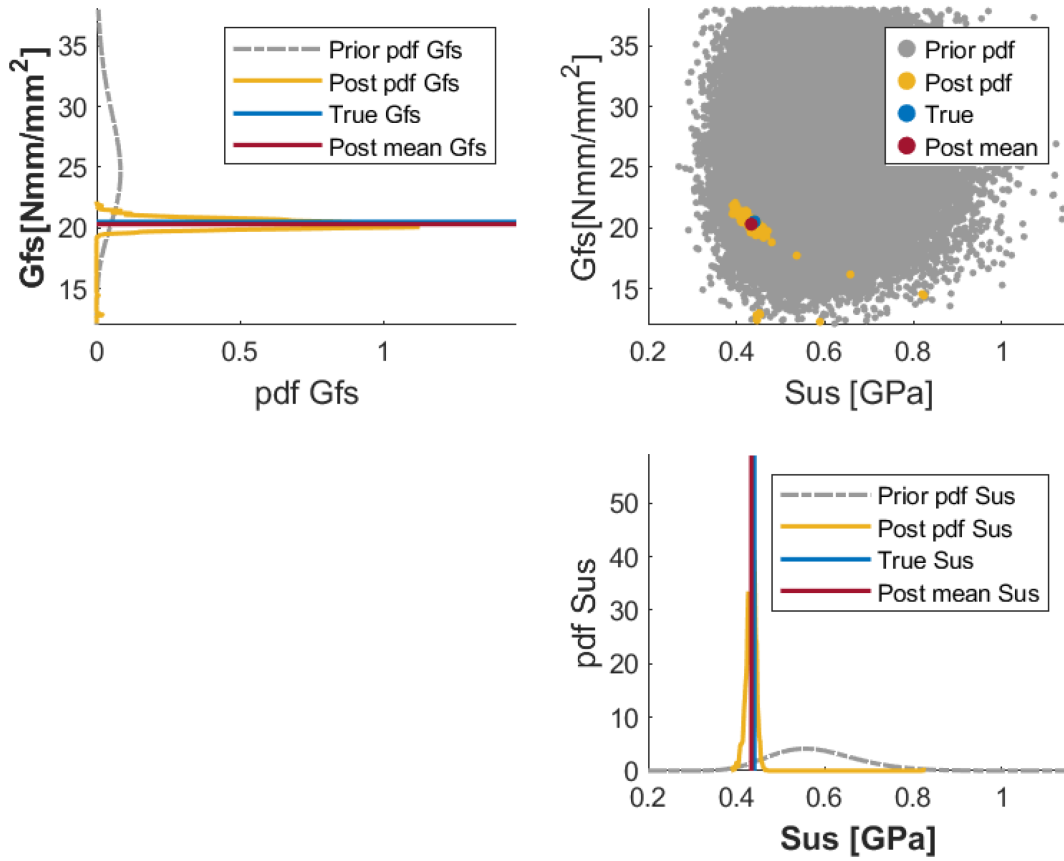


FIGURE 19 | Phase 3 – A-priori distribution of the q_3 parameters and the samples of their a-posteriori distribution, as well as the mean of the posterior samples.

For the corresponding error model, the variances of the covariance matrix C_{E_3} are computed from the following standard deviation

$$\sigma_{E_3} = 0.004 \text{ mm} + \sigma_{\text{proxy},3}. \quad (32)$$

Here, $\sigma_{\text{proxy},3}$ represents the standard deviation of the modeling error introduced by the proxy model in Phase 3.

Figure 19 shows the results of the Bayesian update procedure in the shear phase. The update results in the mean value of $\sigma_{us} = 0.433512$ GPa with standard deviation of 0.0162 GPa. For the shear fracture energy, G_{fs} , the mean value is 20.3137 Nmm²/mm, with standard deviation of 0.6125 Nmm²/mm.

4.6 | Results

In the multiphase stochastic approach, all six unknown material parameters related to dynamic fracture are successfully identified. The results from Kalthoff's test are divided into three phases, with specific measurements taken in each phase to identify a pair of unknown parameters, as outlined in Table 1. Table 5 presents the mean values of the posterior distributions from each phase. Alongside the stochastic method, the “ground truth” with known input parameters was used to assess the accuracy of the identified values. The last column of Table 5 shows the relative difference between the true (correct) values and the computed posterior mean values. The relative difference is generally low, below 1%, except for the shear fracture energy G_{fs} , where the largest difference is 1.6%. This discrepancy arises from the accumulation of errors in the estimated posterior mean values in Phase 1 and Phase 2, which were subsequently used as input data in the following phase(s). This, and the actual realization of measurements errors, led to deviations in the posterior mean values of σ_{us} and G_{fs} in Phase 3. Nevertheless, the results are considered satisfactorily accurate, and all six parameters have been successfully determined.

TABLE 5 | Summary of posterior mean values from the multiphase stochastic identification procedure and comparison with the true values.

Parameter	True model	Phase 1	Phase 2	Phase 3	Difference
K [GPa]	175	175.97	175.97	175.97	0.6%
G [GPa]	80.77	80.65	80.65	80.65	-0.1%
σ_{un} [MPa]	844	—	845.43	845.43	0.2%
G_{fn} [Nmm ² /mm]	22.17	—	22.13	22.13	-0.2%
σ_{us} [MPa]	440	—	—	436.58	-0.8%
G_{fs} [Nmm ² /mm]	20.50	—	—	20.18	-1.6%

5 | Conclusions and Outlook

This study presents a robust multiphase stochastic approach to identify six key material parameters associated with dynamic fracture behaviour. By leveraging Kalthoff's test, we successfully applied a Bayesian updating method to iteratively refine the values of tensile strength, fracture energy, and shear strength across three phases of testing. The use of gPCE surrogate models facilitated efficient exploration of the parameter space, significantly reducing computational costs while maintaining accuracy. Our results show that the identified parameters, with relative differences generally below 1%, are sufficiently precise for practical applications, with the exception of the shear fracture energy, which exhibited a discrepancy of 1.6%. This discrepancy highlights the influence of accumulated errors from earlier phases, but does not undermine the overall success of the methodology. In this study, we relied on synthetic or virtual measurements rather than real experimental data. When using real measurements, the process becomes more challenging due to uncertain modeling errors. However, we also demonstrated here how to address such errors, particularly those arising from the imperfect surrogate model in the low-dimensional space, which also introduced similar errors, thereby presenting a pathway for handling modeling errors effectively. The herein proposed multi-phase approach proved to be an efficient parameter identification method for dynamic fracture mechanics. By the presented analysis we have demonstrated its potential as a tool to support accurate modeling of complex fracture phenomena in engineering applications. Future work will focus on testing the procedure on real experiments, and on the bifurcation problem taking into account the stochastic nature of the forward fracture problem, with the aim of enabling parameter updating for such challenges.

Acknowledgments

Andjelka Stanić gratefully acknowledges support from the Sectorplan Techniek 1, funded by the Dutch Government.

This research has been supported by the project "Parameter estimation framework for fracture propagation problems under extreme mechanical loads" (HRZZ-UIP-2020-02-6693), funded by the Croatian Science Foundation.

The research has also been supported by the project KK.01.1.1.02.0027, co-financed by the Croatian Government and the European Union through the European Regional Development Fund—the Competitiveness and Cohesion Operational Programme.

Hermann Matthies gratefully acknowledges support from a Gay-Lussac Humboldt Research Award.

Noémi Friedman acknowledges the support of the European Commission Horizon Europe project 101092052 BUILDCHAIN and by the European Union project RRF-2.3.121-2022-00004 within the framework of the Artificial Intelligence National Laboratory Program.

Funding

This work was supported by multiple projects, including BUILDCHAIN (Grant No. 101092052), Sectorplan Techniek 1, the Parameter estimation framework for fracture propagation problems under extreme mechanical loads (Grant No. HRZZ-UIP-2020-02-6693), the European Regional Development Fund via the Competitiveness and Cohesion Operational Programme (Grant No. KK.01.1.1.02.0027), and the Artificial Intelligence National Laboratory Program (Grant No. RRF-2.3.121-2022-00004).

Data Availability Statement

The data that support the findings of this study are available on request from the corresponding author. The data are not publicly available due to privacy or ethical restrictions.

Endnotes

¹Variables and quantities denoted with a double overline correspond to the embedded discontinuity Γ^e .

²A random variable or a vector of random variables is denoted by a capital letter, and a specific realization of it by the corresponding lowercase letter.

³In some cases, scaling the projection matrix can be beneficial for stabilizing the surrogate construction and the subsequent updating procedure. This leads to the modified formulation

$$\mathbf{Y}_r = \underbrace{\mathbf{S}_r^{-1} \mathbf{V}_r^T}_{\hat{\mathbf{P}}} (\mathbf{Y} - \boldsymbol{\mu}_Y), \quad (33)$$

where $\mathbf{S}_r$ is the reduced diagonal matrix containing the m_r largest singular values σ_i . This scaling normalizes the reduced variables, yielding unit variance and comparable magnitudes, which can in some situations improve the conditioning of the reduced representation. However, in the examples considered in this work, the standard POD projection without scaling was found to provide more stable and robust MCMC sampling behavior than the scaled formulation.

⁴Later, in our Kalthoff test example, the parameters to be identified have lognormal a-priori distributions. Accordingly, we define $\boldsymbol{\theta}$ as Gaussian random variables obtained by taking the natural logarithm of the lognormal parameters, so that the standard polynomial chaos (PC) expansion can be used for the surrogate model. The procedure is not restricted to Gaussian variables: For parameters with other distributions (e.g., uniform), a generalized polynomial chaos (GPC) expansion with orthogonal polynomials corresponding to the underlying distribution (e.g., Legendre polynomials for uniform) can be applied using the same framework.

⁵In many problems, when the measurable output is high-dimensional, it is often convenient to first train a surrogate model for the full output and then use a low-rank representation of this output before constructing a surrogate for reduced coordinates. However, in this particularly complex case of dynamic fracture problems, the low-rank representation serves an additional purpose beyond facilitating the MCMC updating procedure: It captures the intricate time evolution of the dynamic fracture, thereby improving the accuracy of the surrogate. For this reason, we do not construct a surrogate in the full-dimensional representation. Consequently, the covariance matrix—which in simpler cases could be directly computed from the GPC coefficients—must instead be evaluated from samples of the response. Due to the high complexity of the problem, a large number of samples is required for training the surrogate anyway, making this approach computationally feasible.

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