Bayesian inversion with open-source codes for various one-dimensional model problems in computational mechanics

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Nima Noii[a] Amirreza Khodadadian[b] Jacinto Ulloa[c], Fadi Aldakheel[a,d,1]
Thomas Wick[b,e,f], Stijn François[c], Peter Wriggers[a,e]

[a] Institute of Continuum Mechanics
Leibniz Universität Hannover, An der Universität 1, 30823 Garbsen, Germany

[b] Institute of Applied Mathematics
Leibniz Universität Hannover, Welfengarten 1, 30167 Hannover, Germany

[c] Department of Civil Engineering
KU Leuven, Kasteelpark Arenberg 40, 3001 Leuven, Belgium

[d] Zienkiewicz Centre for Computational Engineering, Faculty of Science and Engineering
Swansea University, Bay Campus, SA1 8EN, UK

[e] Cluster of Excellence PhoenixD (Photonics, Optics, and Engineering - Innovation Across Disciplines) Leibniz Universität Hannover, Germany

[f] Université Paris-Saclay, ENS Paris-Saclay
LMT – Laboratoire de Mécanique et Technologie, 91190 Gif-sur-Yvette, France

Abstract

The complexity of many problems in computational mechanics calls for reliable programming codes and accurate simulation systems. Typically, simulation responses strongly depend on material and model parameters, where one distinguishes between backward and forward models. Providing reliable information for the material/model parameters, enables us to calibrate the forward model (e.g., a system of PDEs). Markov chain Monte Carlo methods are efficient computational techniques to estimate the posterior density of the parameters. In the present study, we employ Bayesian inversion for several mechanical problems and study its applicability to enhance the model accuracy. Seven different boundary value problems in coupled multi-field (and multi-physics) systems are presented. To provide a comprehensive study, both rate-dependent and rate-independent equations are considered. Moreover, open source codes are provided, constituting a convenient platform for future developments for, e.g., multi-field coupled problems. The developed package is written in MATLAB and provides useful information about mechanical model problems and the backward Bayesian inversion setting.

Keywords: Open-source codes; elastoplasticity; phase-field fracture; thermoelasticity; fatigue failure; Bayesian inversion

[1]Corresponding author.

E-mail addresses: noii@ikm.uni-hannover.de (N. Noii); khodadadian@ifam.uni-hannover.de(A. Khodadadian); jacintoisrael.ulloa@kuleuven.be(J. Ulloa); aldakheel@ikm.uni-hannover.de (F. Aldakheel); thomas.wick@ifam.uni-hannover.de (T. Wick); stijn.francois@kuleuven.be (S. François); wriggers@ikm.uni-hannover.de (P. Wriggers).

Table 1: The overview of the Bayesian inversion codes.

Code	description
`MH.m`	the Metropolis-Hastings techniques
`AMH.m`	the adaptive Metropolis
`MH_DR.m`	the delayed rejection Metropolis
`DRAM.m`	the delayed rejection adaptive Metropolis technique
`EnKF.m`	the EnKF-MCMC method
`check_bound.m`	adjust the proposals according to the given upper/lower bounds
`covupd.m`	adaptation of covariance function
`prior.m`	the generation of the uniform prior distribution
`EES.m`	the computation of square error

1. Overview software package

Bayesian inversion is a robust, simple, and efficient computational technique to provide reliable information about the model parameters and uncertainties. The mechanical models given in this work constitute relevant model problems that can be further considered in further works. The provided codes can be introduced/discussed in academic classes and can be extended to two- or three-dimensional settings. Moreover, the given examples have been considered in recent fundamental and applied studies. Of course, there are still several open questions in these fields, and we hope that the codes provided herein can be a starting point for further researches

In this documentation, we present an overview of the codes and discuss their performance as the forward and backward models. Here, we strive to provide a comprehensive package to review the common MCMC techniques. Table 1 shows the MCMC codes including their description. We should note that in all examples the function `forwardmodel.m` is the forward model and considers the response of the model problem to the given candidates. An overview of the mechanical codes is given in Table 2.

We observed that for the problems with one unknown, all MCMC techniques worked efficiently. Similar results have been achieved for a two-dimensional probabilistic problem, in case that the parameters do not correlate (heat problem). For more complicated examples, MH, AMH, and DR were not effective; therefore, DRAM and EnKF have been employed. Due to the more efficient proposal adaptation when using the Kalman filter, the acceptance rate is noticeably higher compared to DRAM. EnKF works well for phase-field problems, including brittle and ductile fracture. The obtained results for fatigue fracture were not as good as for other examples, likely due to the high correlation of the critical fracture and fatigue parameters.

Table 2: The overview of the one-dimensional mechanical codes.

Code	example	description
elasticity_1D.m	Example 1	the main script to infer E
linelast.m	Example 1	computation of the elasticity
heat_1D.m	Example 2	the main script to infer κ and $\mathcal{K}$
EP_1D.m	Example 3	the main script to infer E, H, and σ_Y
Global_stiffness_Initial_cal.m	Example 3	calculation of the stiffness matrix force vector in elastoplastic deformation
brittle_1D.m	Example 4	the main script to infer E and G_c
elasticity_PDE.m	Example 4	elasticity equation in brittle fracture
phase_field_PDE.m	Example 4	phase-field equation in brittle fracture
ductile_1D.m	Example 5	the main script to infer E, σ_Y, w_0, and H
elasticity_PDE.m	Example 5	elasticity equation in ductile fracture
plasticity_PDE.m	Example 5	plasticity equation in ductile fracture
phase_field_PDE.m	Example 5	phase-field equation in ductile fracture
thermoelastic_1D.m	Example 6	the main script to infer G_c, E, K, and α
elasticity_PDE.m	Example 6	elasticity equation in thermoelastic fracture
plasticity_thermal.m	Example 6	thermal equation in thermoelastic fracture
phase_field_PDE.m	Example 6	phase-field equation in thermoelastic fracture
fatigue_1D.m	Example 7	the main script to infer E, k, G_c, and γ_c
elasticity_PDE.m	Example 7	elasticity equation in fatigue failure
phase_field_PDE.m	Example 7	phase-field equation in fatigue failure