Accepted Manuscript

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PII: S0266-8920(16)30161-8
DOI: https://doi.org/10.1016/j.probengmech.2017.10.003
Reference: PREM 2946

To appear in: *Probabilistic Engineering Mechanics*

Received date : 5 November 2016
Revised date : 26 September 2017
Accepted date : 18 October 2017

Please cite this article as: M.F. Badawy, M.A. Msekh, K.M. Hamdia, M.K. Steiner, T. Lahmer, T. Rabczuk, Hybrid nonlinear surrogate models for fracture behavior of polymeric nanocomposites, *Probabilistic Engineering Mechanics* (2017), https://doi.org/10.1016/j.probengmech.2017.10.003

Hybrid nonlinear surrogate models for fracture behavior of polymeric nanocomposites

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Abstract

We present a hybrid nonlinear surrogate model for fracture in polymeric nanocomposites. The phase field method is employed to model fracture in the polymer matrix. Since the stochastic analysis on the output of the mechanical model is prohibitively expensive, surrogate models (SM) are very attractive alternatives. In order to get an optimal and robust solution, we propose a hybrid nonlinear surrogate model (HSM) for the prediction of the fracture toughness of PNC. It is constructed with the use of the polynomial regression and the Kriging interpolation. The support data for such HSM is generated by a phase-field model for brittle fracture with six chosen input parameters. The validation of the surrogate model and by this its qualitative assessment is done based on a scanning test set algorithm. The constructed and assessed HSM is then used to present the behavior of fracture toughness of PNC with respect to various input parameters with very low computational costs and high accuracy. Within the domain of interest, the analysis shows that Young's modulus of the matrix has no optimum value, in which, the higher input value causes higher response. On the other hand the volume fraction of clay platelets at about 5% showed stability of the response, in which, the higher input value leads to no change in the response.

Keywords: Polymer nanocomposites, phase-field model, brittle fracture, surrogate model, cross-validation

1. Introduction

In the last decades, intensive studies have been carried out in order to predict the behavior of polymeric nanocomposites (PNC). Particularly challenging is the prediction of fracture related properties due to the complex microstructure, size effects and the high computational cost. For example, the reference numerical model in the current study consisting of 20,512 elements requires a CPU time of about six hours on a 4 $\times$ Twelve-Core AMD Opteron^{TM} Processor of HP ProLiant DL585 G7 system.

A single numerical simulation can provide information about only one point in the domain, accordingly a global understanding for the fracture behavior of PNCs, within the limits of a finite domain based on numerical simulations, can solely achieved by the aid of SM. On the other side, due to the long running times and the lack of analytic gradients, almost all optimization algorithms applied directly to numerical simulation are computational wise very expensive. Accordingly, surrogate-based optimization [1] have been developed and broadly expanded. This also applies in case of sensitivity analysis (specially for PNC as discussed in the literature [2]) and reliability analysis. Moreover fracture behavior of PNC is a multidimensional problem, accordingly an adequate descritization method is required to achieve an acceptable understanding of the entire domain. Uniform mesh-grid, Monte Carlo simulations, Latin-hypercube

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