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ASSESSING UNCERTAINTY IN CREEP LIFE OF GRADE 91 STEEL USING CRYSTAL PLASTICITY AND GRAIN BOUNDARY MICROSTRUCTURAL MODELS

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Abstract
This paper examines time to minimum creep rate and its uncertainty with respect to a set of fourteen material parameters. The microstructural model of Grade 91 steel includes both dislocation creep and grain boundary opening/sliding within a finite element model, and hence the simulations are relatively expensive and have several sources of nonlinearity. We will propagate uncertainty in the input material parameters of these two mechanisms and determine the aggregate uncertainty in the predicted time to minimum creep rate as well as the sensitivities of the parameters. The cost, stability, accuracy of the polynomial chaos expansion as a means for stochastic dimensional reduction is assessed against the classical Monte Carlo method.

1. Introduction

Creep performance in Cr-1Mo-V alloy (Grade 91) has been crucial in the design of high temperature structural components in fossil, gas or nuclear power plants, and the aim has been toward higher operating temperatures to improve performance. Thereby, creep failure is a concern in designing these components as the target design lifespan for modern plants is more than 60 years, for which direct test data does not exist. In creep test data, there is a lot of experiment-to-experiment and heat-to-heat variability, and understanding that variation could help the engineers design components to account for that uncertainty. Nassif et al developed a microstructural model for creep in Grade 91 ferritic-martensitic steel considering the deformation mechanisms from dislocation, diffusional motion within the prior austenite grains, viscous sliding and cavity growth, and nucleation along grain boundaries. Solid and interface finite elements are incorporated into the WARP3D code to explicitly capture these behaviors in the Grade 91 microstructure.

The reliability of numerical models as surrogates to real world problems is established through the concept of uncertainty quantification, where non-deterministic approaches are utilized to evaluate a system that is subjected to a range of variable inputs. Monte Carlo (MC) method is considered a sampling-based technique and its numerical cost is relative to the standard deviation of the quantity of interest (QoI) that is unknown until the end of simulation. On the other hand, non-sampling methods like polynomial chaos expansion (PCE) provide the ability of explicitly mapping input random variables to the output QoI, allowing for a prompt and exhaustive sensitivity analysis.

2. Results

This project takes advantage of deep neural network as a surrogate to the crystal plasticity finite element model of Nassif et al. for Grade 91 steel, and the non-intrusive generalized polynomial chaos expansion to create a methodology to investigate the uncertainty quantification of highly nonlinear models with multiple dimensions. This surrogate model is cheap to evaluate after being trained with a moderate number of simulations, and its accuracy is relatively high. Then the surrogate model is used to perform sensitivity analysis to calculate the Sobol indices, and the Sobol indices are used to reduce the dimensionality of the problem by eliminating the parameters that do not contribute to the variation of the QoI. The reduced models are used to perform the uncertainty quantification through the generalized polynomial chaos expansion (gPCE), and the results are compared to the results of MC simulation of the original model and the reduced ones. There are a few packages available to use for performing the gPCE. In this study, DAKOTA and ChaosPy were used to generate the sparse grid approximation for the input distributions. The gPCE method's hyperparameters, such as polynomial degree and sparse grid level, as well as the dimensionality of the problem, all have an impact on the validity of the surrogate model and must be properly tuned. To discover the best hyperparameters for this problem, a grid search study was carried out.

One of the simple and common methods of sensitivity analysis is to change one factor at a time and observe its effect on the output, known as one-at-a-time sensitivity analysis (OAT). For this purpose, we set up a study where each variable is set once as its minimum value and once at its maximum value while the other ones are kept at their mean. Table 1 presents the 16 parameters each with their minimum, mean, and maximum value. These bounds were derived by assuming that the actual variation in the parameters would be less than what would be expected for a 100º C difference in temperature. Figure 2 shows the total creep rate versus time for various cases in which a parameter is considered as min (Figure 2) or max (Figure 2b) and others kept at mean value.

Table 1. The CPFE model input parameters and their range of variation

Parameter	E	ν	τ_y	τ_v	n	γ	θ_0	D_η
min	156750	0.294	28	8	11	9.00E-08	750	1.50E-10
mean	165000	0.309	40	12	12	9.55E-08	800	1.20E-09
max	173250	0.324	52	16	13	1.00E-07	850	7.00E-09
Parameter	η_0	K_n	a_0	b_0	D	Ψ	$\sum_0$	F_N/N_I
min	3.00E+05	1.00E+08	5.00E-05	5.00E-03	2.00E-16	75	50	1.00E+04
mean	1.00E+06	1.00E+08	5.00E-04	5.00E-02	1.00E-15	75	525	2.00E+04
max	4.00E+06	1.00E+08	1.00E-03	1.00E-01	3.00E-15	75	1000	9.00E+04

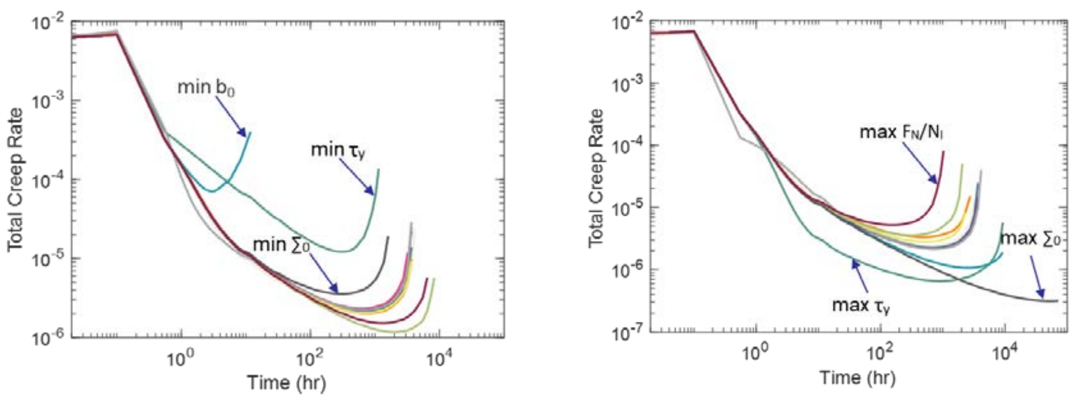

Figure 1. Creep rate figures for different OAT cases, a) Minimum of the range for each parameter, b) Maximum of the range for each parameter

3. Conclusions

The result for mean and standard deviation (SD) of time to minimum creep for the MC and gPCE analyses conducted using the surrogate model are listed in Table 3. The MC analyses used 10000 samples in each case, such that the gPCE method was found to provide similar accuracy with fewer samples. Also, the majority of the distribution in time to minimum creep is attributed to 6 parameters; further reduction impacted the accuracy of the quantified uncertainty.

Table 3. The Monte Carlo method and gPCE method uncertainty quantification results

Dims	**Mean**	**SD**	**Dims**	**Number of points**	**Mean**	**SD**
14	4.19	0.60	14	5573	4.19	0.61
6	4.18	0.59	6	689	4.19	0.58
3	4.15	0.55	3	147	4.15	0.54