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Identification of best fit parameters of void nucleation and growth model using particle swarm technique

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ABSTRACT

The void nucleation and growth (NAG) model describes fracture as a result of nucleation and growth of voids in the ductile materials at the microscopic scales. This model involves five material-dependent parameters, best-fit values of which must be determined by matching with atomistic simulations (MD). This is done by minimizing the difference between the temporal evolution of void volume yielded by MD and by the NAG model. The NAG model represents a real valued, non-linear and non-continuous optimization problem. Therefore, an swarm intelligence based technique, particle swarm optimization (PSO) is used for optimum parameters search. The search algorithm is developed on PSO to iteratively search optimum point, starting with a given reference search space and improving it based on the location of best searched point in each iteration. The PSO code is developed using object oriented design patterns so that the same can be extended for other materials without a base change. The paper discusses the code details, best fit parameters for Niobium (Nb) and Molybdenum (Mo) crystals and algorithmic parameters tuning of the modified algorithm. It has been shown that parameter tuning has shown improved results in terms of lower computing cost. It is seen that the MD results match the NAG model with a root mean square error of 7% and 15% for perfect crystal Nb and Mo and 10% and 17% for Nb and Mo crystal with edge dislocation, respectively. Novel features of the work includes the systematic movement of search-space boundaries to aid convergence in an unknown search-space. The sensitivity of the best result to algorithmic parameters and comparative analysis against other PSO variants has also been studied.

1. Introduction

1.1. Fracture model

Hydrodynamic codes modeling shock waves, high velocity impact and penetration requires, as a critical input, the fracture properties of solid. These are specified through a fracture model such as the void nucleation and growth (NAG) model [1,2], which quantifies the rate of nucleation and growth of voids in a solid. This model is defined in terms of total void volume due to nucleation and growth of voids and has five material dependent parameters. A multi scale model for single crystal spallation at high strain rates [3] uses MD simulations at the atomic scales to deform a solid by isotropic, tri-axial tension. This leads to nucleation, and subsequently growth and coalescence of voids, which is an output of the MD simulations. The best fit parameters of the NAG model can be obtained by fitting to the results of the MD simulations. The best fit parameters for Copper (Cu) [4] have been obtained using this approach. Nb and Mo are the materials used for development of structural components of fusion and nuclear engineering devices. This approach of obtaining optimized values for NAG from MD data is useful. It aids in understanding the fracture behavior of Nb and Mo under high strain rates. A multi scale model for crystal spallation at high strain rate is shown in Fig. 1.

1.2. Problem description

1.2.1. Numerical model

The nucleation and growth model [1,2] developed at Standford Research Institute, is a micro physics model which describes the fracture process as a result of void nucleation and growth in a ductile material. The voids are created when the tensile pressure P_s in the solid exceeds the nucleation threshold of the material P_{no}. The nucleation rate of voids $\dot{N}$ is given by

$$\dot{N} = \dot{N}_0 \exp\left[\frac{P_s - P_{n0}}{P_1}\right], \quad P_s > P_{n0} \tag{1}$$

$$\dot{N} = 0, \quad P_s \leq P_{n0} \tag{2}$$

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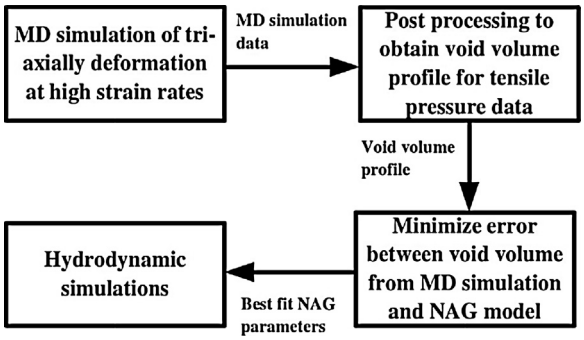

Fig. 1. Multi scale fracture model.

where P_1 is the pressure sensitivity of the material for void formation and P_{g0} is the growth threshold for voids. The volume of void nucleated is given by

$$\Delta V_n = 8\pi \dot{N} \Delta t R_n^3 \tag{3}$$

where R_n is a material parameter known as nucleation size parameter. We take it as initial size of the nucleated void. The void volume increase due to growth of existing voids is given by

$$V_g = V_{vo} \exp\left[\frac{3}{4}\left(\frac{P_s - P_{g0}}{\eta}\right)\right] \Delta t \tag{4}$$

where η is the material viscosity and V_{vo} is the void volume at the beginning of time interval. The void volume due to nucleation and growth of void at the end of time interval is given by

$$V_{NAG} = \Delta V_n + V_g \tag{5}$$

we define two sets of volumes, V_{NAG}, a set of values calculated from the NAG model and V_{MD}, a set of values calculated from the MD simulations. The relative error (ϕ) of the fit to the MD data thus is given by

$$\phi = \sum \left[\frac{V_{NAG} - V_{MD}}{V_{NAG}}\right] \tag{6}$$

The root mean square error (ϵ) is given by

$$\epsilon = \sqrt{\left[\frac{(\phi)^2}{N}\right]} \tag{7}$$

1.2.2. Objective function and complexities

The objective function is given by

$$\underset{\dot{N}, P_1, P_{n0}, P_{g0}, \eta}{\text{Minimize}} \quad \epsilon \tag{8}$$

From the MD simulation results a rough idea of the upper bond of P_{n0} and the lower bound of P_{g0} can be obtained. The range and value of the other three variables depend on the range of these two parameters. A conjugate gradient based search algorithm which was used for fitting the NAG parameters yielded large error (>30%) when fitted to the MD results. The uncertainty in range and large errors, indicate that an algorithm like PSO can be used to explore the parameter space and if needed extend the search space dynamically as part of the algorithm to obtain a better match with the MD results. We made following observations from Eq. (8):

1. The objective function is a non-linear, exponential function in a five-dimensional hyper-space. It is very sensitive to it's input variables and a small change in inputs make a huge change in the void volume.
2. Typically, material deformation fracture models have a very steep global minima.
3. We do not have an accurate predication of the search space for the problem. We have a reference search space for the above objective problem.
4. Since the data are taken from the atomistic MD simulation, the parameters attains very high values of the real numbers.
5. During testing of the objective function, we observed that it also provides the NaN (non-computable) values for parameter regions which makes it unsuitable for gradient based optimization algorithms.

In this paper, reported work is driven by the following objectives:

1. Searching for a good reference space.
2. Optimize the objective function and obtain best fit parameters.
3. Tuning of the algorithmic parameters to save on computational cost.

2. Literature survey and optimization strategy

2.1. Nature-inspired algorithms and motivation for selection of PSO

Nature inspired algorithms are widely used to solve the real world optimization problems. These algorithms are based on evolution and emulation of the nature-inspired intelligence approaches for the problem solving. These algorithms are widely used in situations where conventional gradient based algorithms cannot be applied or not efficient to implement [5–10]. These algorithms are broadly classified into four categories as defined in [11] on the basis of source of inspiration as: (1) swarm intelligence based, (2) bio-inspired (but nonswarm intelligence based), (3) physics/chemistry based and (4) others. Few of the most popular algorithms are: genetic algorithms (GA) [12], PSO [13], differential evolution (DE) [14], ant colony optimization [15], evolution programming (EP) and evolution strategies (ES). The researchers have compared the performance of natured inspired algorithms on various optimization problems and standard analytical benchmark functions [16–18]. It has been found that although there is no thumb rule in general for all the optimization problems but PSO is found to be a simple in implementation yet comparatively efficient technique. PSO is based on the concept of swarm intelligence. Its rapid convergence and small computational time make it a good candidate for solving high dimensional optimization problems. In summary, the following reasons motivate us to use PSO technique:

1. PSO is easy to implement and gradient free.
2. PSO has few algorithmic parameters to be tuned.
3. PSO algorithms are defined inherently for n-dimensional search space. In case the model is enhanced from it's five-dimensional form then no significant modification is needed in the algorithm.
4. PSO is a valuable technique to find optima in a fitness landscape and is especially useful when dealing with a high number of dimensions and problems where problem specific information does not completely and sufficiently exist.
5. PSO technique has a vast data base of published applications [19,20].
6. Computational fracture modeling is a new application area for PSO although PSO is a proven performer for benchmark functions [21,16–18].