Optimization Strategies for Parameter Estimation in Constitutive Models

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Abstract
Prediction of a material’s mechanical response under external load relies on the correctness of the constitutive model being used. The constitutive equations contain a number of adjustable parameters and, depending on the internal state variables considered, can be broadly classified as “physics based” or “phenomenological based”. Typically, with reduced crystal symmetry the number of these adjustable parameters increases, rendering a purely empirical estimation largely unfeasible. Therefore, an efficient optimization strategy is required to estimate these parameters. Currently, the Nelder–Mead (NM) simplex method is predominantly used to optimize the constitutive parameters based on an inverse computational scheme that compares experimental results to corresponding simulations. The simplex method has, however, shortcomings as it always converges to the nearest local minimum.

Particle Swarm Optimization algorithm is investigated as an alternative strategy for constitutive parameter estimation of highly anisotropic systems embedded into an overall architecture for systematic identification of constitutive parameters.

Constitutive law: Phenomenological Power Law
Physics based models generally use dislocation density as their state variable whereas phenomenological models are based on critical resolved shear stress per each slip system and are mostly used because of their apparent simplicity. One exemplary phenomenological model is due to Peirce et al. [1]:
• The plastic deformation rate (plastic velocity gradient) is related to the shear rate on individual slip systems
  \[ \dot{\gamma} = \sum_{i=1}^{N_s} \dot{\gamma}_i^m \otimes n^m \]
  \( \dot{\gamma} \) is shear rate on individual slip systems
  \( \gamma^m \) is the m-th component of the critical resolved shear stress
  \( n^m \) is the m-th component of the slip direction

• Shear rate on individual slip systems is following a power law kinetics

• The hardening (change of critical resolved shear stress) is linked to shear on all slip systems
  \[ \tau^c = q_{0c} \left[ n_0 \left( \frac{T_n}{c_s} \right)^{\frac{m}{n}} \right] \]

Thus for each slip family we have a set of constitutive parameters, \( \eta_0, \gamma_0, m, n_0, T_n, c_s \) and \( q_{0c} \) which control the overall response and hence the predictive capability of the model.

Methodology
The overall architecture of systematic identification of constitutive parameters is shown. The importance of an efficient optimization strategy is evident, especially for non-cubic crystal systems having large parameter space.

Particle Swarm Optimization
Particle Swarm Optimization (PSO) is a stochastic optimization technique based on the principle of randomization. Essentially a set of random particles are initiated and their positions are updated based on two attracting points local_best and global_best. In conventional PSO algorithms the particles are mass-less with only initial velocities and their motion is governed by their distances from these two attractors as well as their individual spring constants (social factors).

Convergence tests of PSO and NM simplex algorithms

Advantages of PSO
• PSO is preferred to other evolutionary algorithms as it doesn’t require the evaluation of the gradient.
• Has a higher probability of converging to a global minimum.
• Is efficient for optimizing multi-modal functions.

Disadvantages
• Computationally more intensive than NM simplex method and hence has to made efficient by suitable modifications.
• The theoretical foundation is weak and needs more exploration [3].

Discussion
It can be seen that NM simplex method requires lesser function evaluations to reach towards the optimum solution than PSO, but the converged solution itself becomes questionable at times. Development of PSO in terms of function evaluations would undoubtedly decrease its computation cost and its incorporation to evaluate adjustable constitutive parameters would definitely increase the correctness of model.

References