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Modeling elasto-viscoplasticity in a consistent phase field framework

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Summary on the novelties in our manuscript

1) **Formulated a thermodynamically consistent phase-field theory for elasto-viscoplasticty**
   1.1) **It provides a way to improve and generalize Guo's phase-field model that has been widely cited.** Guo et al. only minimizes the shear part of strain energy (disregard the hydrostatic part) and only deals with perfect plasticity, which is shown to be not thermodynamically consistent and its application is limited. We can treat general isotropic hardening and provided justification.
   1.2) **Recovered classical plasticity laws such as Prandtl-Reuss and Odquivist's law through the kinetic equation of phase field (TDGL type equation) with minimal assumptions**. These classical plasticity laws are derived based on assumptions of *(a) association plasticity and normality and (b) von Mises load function or a priori postulated dissipation potential*. These assumptions are opaque to phase field modeling, but are not used in our derivation. We instead go through the standard phase-field procedure, by defining free energy and minimizing it through constrained variational principle and the TDGL type equation. In addition, we justified (thermodynamic allowance) the choice of the tensor kinetic coefficient and there is a possibility to derive different (new) flow rules provided there is experimental support.
   1.3) **This theory paves the way for coupling plastic flow with microstructural evolution through total free energy rather than merely through total strain.** In existing phase-field models that directly employ classical plasticity theories, the two parts (phase-field and plasticity) can only be linked through total strain, and other than that they are *black boxes* to each other.

   ** Whether plastic strain can be called order parameter, whether our kinetic equation can be called TDGL equation, or whether our model itself can be called phase-field theory, should not be important. The above 3 points hold even if we change the terminology. However, we have provided sufficient justification for our model to bear the names.*

2) **The three-dimensional model is systematically validated by a series of analytical solutions (and it shows excellent parallel efficiency)**
   2.1) We **systematically** simulated an expanding inclusion in elastoplastic matrix with perfect plasticity, linear strain hardening, and power-law strain hardening and compared results with analytical solutions and numerical solution of other authors. In addition, we formulated J-integral based on Khachaturyan's theory and calculated J of a Mode I crack in different regimes. **All simulation results are in excellent agreements with analytical solutions or theoretical predictions.** These analytical solutions could be used as benchmark for other numerical tools.
   2.2) We extended Wang's algorithm (in pure elastic regime) to treat free surface in elastoplastic regime, and in the mean time we develop an analytical solution for inclusion in a plastic matrix with finite radius. **The analytical solution validates our model, which means our FFT based model can treat free external surface without artificial effects caused by the periodic boundary condition** (important for simulating isolated particles, rods and sheets).