Phase-field Dislocation Dynamics Code Optimization

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The importance of the study of nanocrystalline materials has gained a huge amount of attention these years due to its extraordinary mechanical, electrical and chemical properties. One significant way to progress in this field is by simulating the behavior of the particles in nano scale, which is not only a need but a challenge due to massive interactions that occur there. The phase-field dislocation dynamics (PFDD) method has been successfully employed in the modeling of plastic deformation, creep and grain boundary sliding. In PFDD, the plastic strain and the energy are functions of phase fields that obey a set of complex equations. In the algorithm approach this complexity increases depending on different factors that, in the end, increase the time and computational resource used, which this research pretend optimize. Even though Fast Fourier Transformation and MPI have been utilized in the PFDD code due to his optimal approach and matricial representation which makes the algorithms more understandable the efficiency is still a major concern in matters of computational time and resource consumption. This research intends to give an improvement to the programs that simulates the nanocrystalline materials and the models that follows the dynamics locations so outgoing researchers can use it in a more efficient way. The result will be a improved program that follows the PFDD models and simulates the nanocrystalline behavior with different materials and different constraints in the environment as in the materials itselfs with a more friendly and intelligent input for the user.