1096-65-1380 **Maria Emelianenko*** (memelian@gmu.edu), **Claudio Torres** and **Dmitry Golovaty**.

Computational modeling of polycrystals: accuracy and sensitivity analysis.

The study of the effect of various microscopic features on the meso- and macroscopic behavior of polycrystalline materials undergoing coarsening has received a lot of attention due its extreme importance in technological applications. From computational point of view, various numerical simulation models exist to date, but little has been done so far to investigate the effect of numerical and modeling parameters on the statistics generated by these codes. In fact, very often numerical limitations of such models are not rigorously investigated, which puts them at risk of producing inaccurate predictions. This work represents the first attempt to fill this gap by conducting a thorough numerical investigation of a set of 2-d grain growth simulation models called vertex models, as well as some related 1-d models. This study sheds light onto several important questions, such as whether or not statistics is affected by the choice of grid resolution, grain boundary flipping rules and dynamical features of the model. Rigorous estimates of the flipping rates and steady state distributions are also obtained. Extensive comparison is performed against numerical codes available in the literature as well as experimental data, for both isotropic and anisotropic grain boundary energy. (Received September 15, 2013)