Generation of realistic polycrystalline structure

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04 July 2018

Introduction

The three-dimensional polycrystalline models with the log-normal grain size distribution are constructed by constrained Voronoi tessellation. For achieving needed distribution of grain sizes and grain orientation I used Genetic Algorithm (GA) with Least Square (LS). GA is also used for achieving realistic distribution for grain orientation distribution. Molecular-dynamics method is used in LAMMPS simulation software to obtain the relaxed polycrystal. For the relaxation process and for simulation multibody potential (embeded atom method) is used.

Main idea

There are known a lot of modern application of polycristalline materials. Polycristallines are used for tritium generation [1], automotive, healthcare and non-destructive testing [2], solar cells [3], semiconducting elements [4] etc. With increasing demand of new properties of new materials increases also need for the modern methods of polycristalline simulation [7]. And this work is one more attempt to deal with the simulation of polycryrstallines in molecular dynamics environment such as LAMMPS [5, 6]. The main idea is to build some solid complete methodology in order to build realistic polyctstalline structure in some meaningful time. By saying realistic structure I mean structure that correspond real grain characteristics like grain size distribution and grain orientation distribution.

Grain size

As a pilar for this work the study of Shen [7] is used. Especially idea of using GA for achieving needed grain size distribution. In our case it is lognormal distribution:

$$f(x) = \frac{1}{x}\frac{1}{\sigma\sqrt{2\pi}} exp(-\frac{(ln(x)-\mu)^2}{2\sigma^2}) \quad (1)$$

In order to find better solution there were implemented several crossover and mutation operators. Several parameters were extracted from the operators implementation in order to control evolution process. For building Voronoi tessellation Voro++ library is used.

Methodology

Each individual is container with 3D points (seeds) inside. Genome of individual is coords of seeds. We need to implement operators over this set.

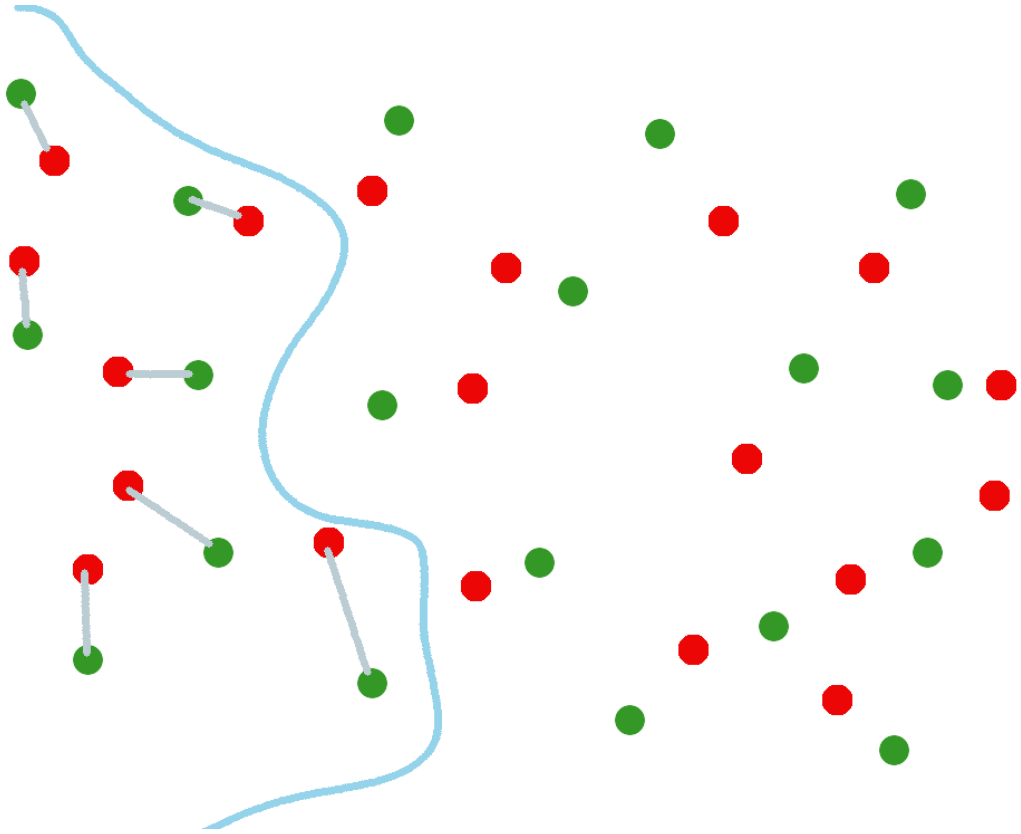

Figure 1: Cross section surface is now defined according to the seed-seed mapping

Methodology

12 parameters needed to be tested in order to find best set of parameters. Here just on example of comparison of values. Mutation probability and population size.

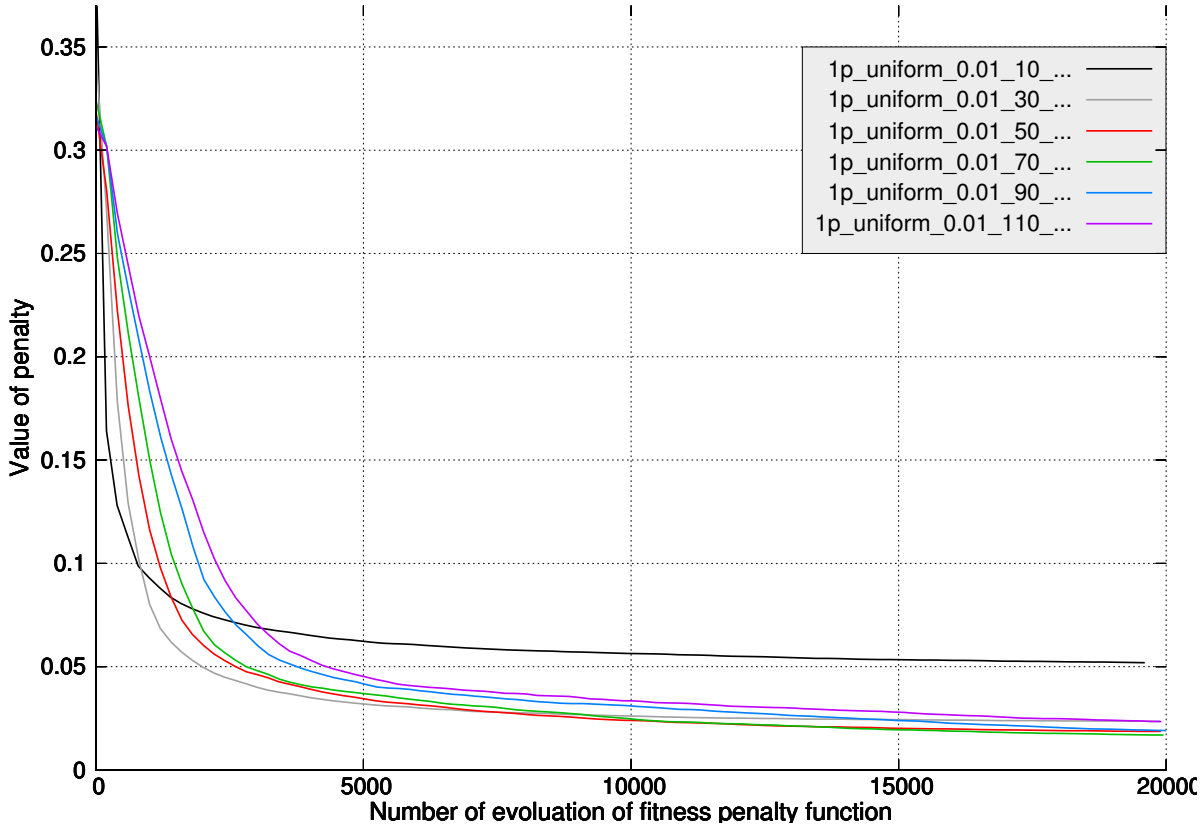

Figure 2: Comparison of mutation probability with population size

Methodology

Some of parameters are compared just approximately by comparing graphs.

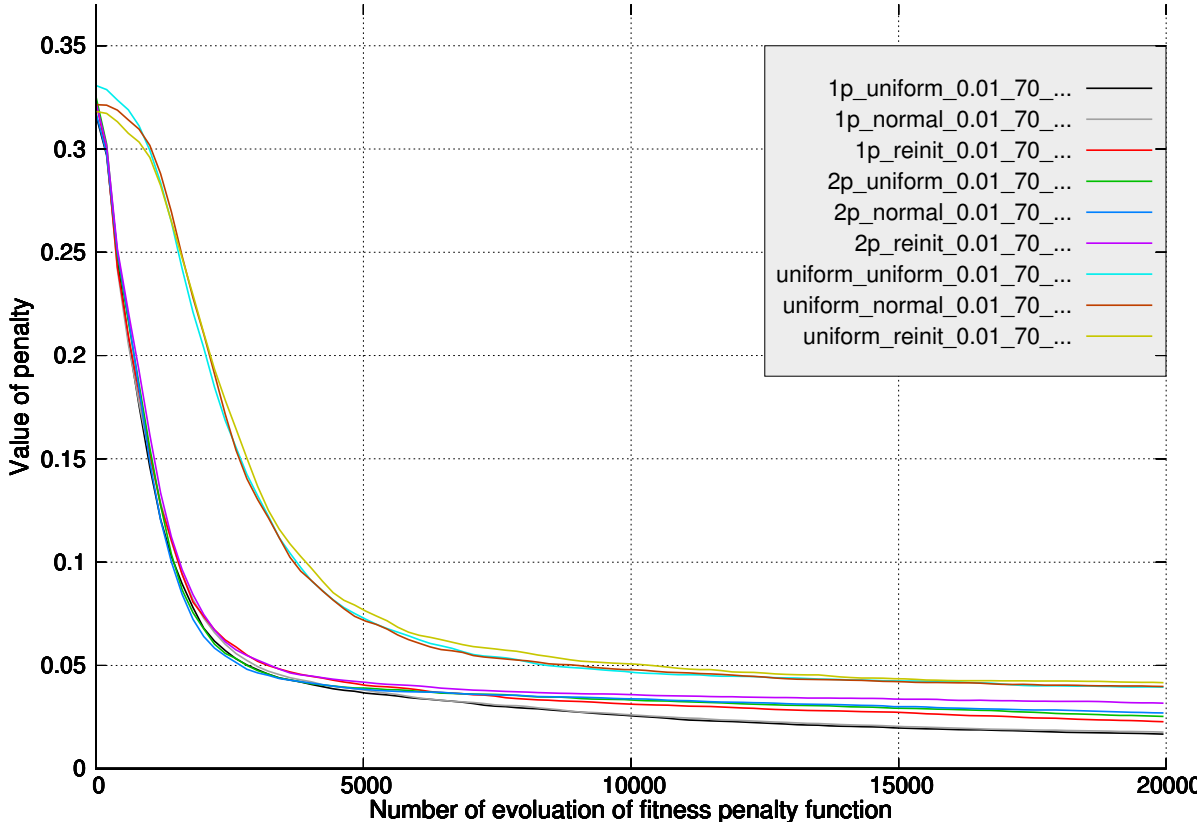

Figure 3: Comparison of different implementations of operators

Methodology

But some parameters compared analytically like mutation probability and population size. For this we divided penalty evolution graph into two parts and fitted data to some functions. Then we introduced measure to select best configuration.

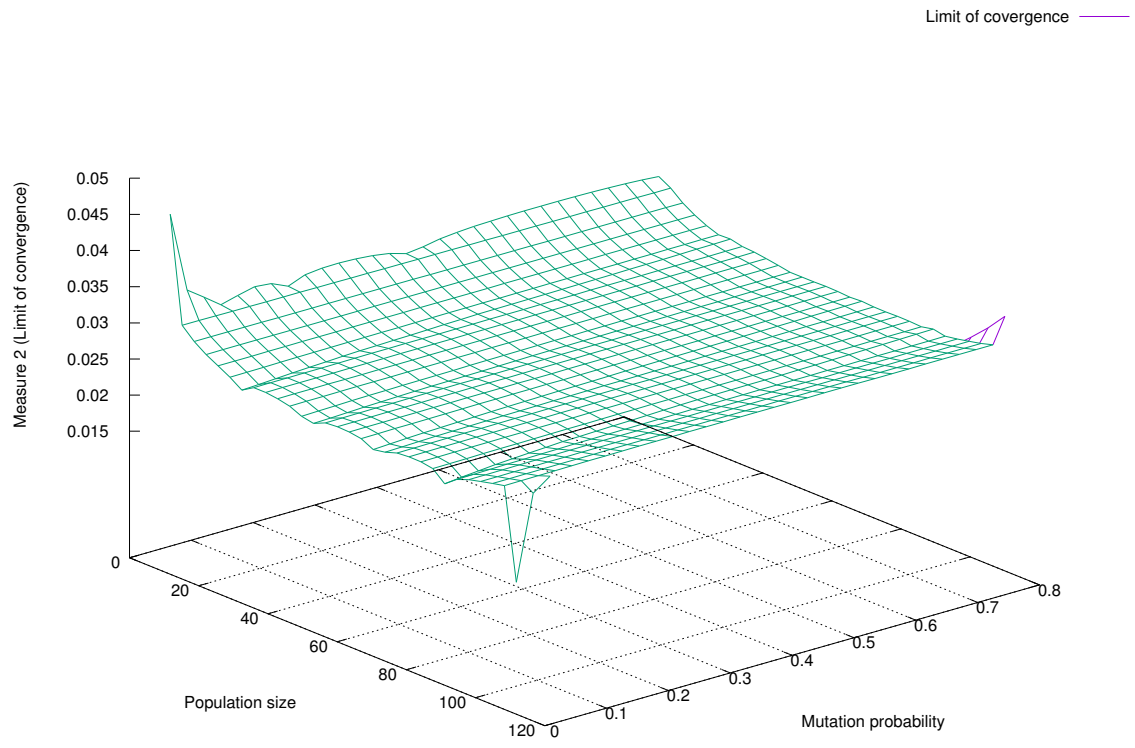

Figure 4: Surface of measure for second part of graph

Methodology

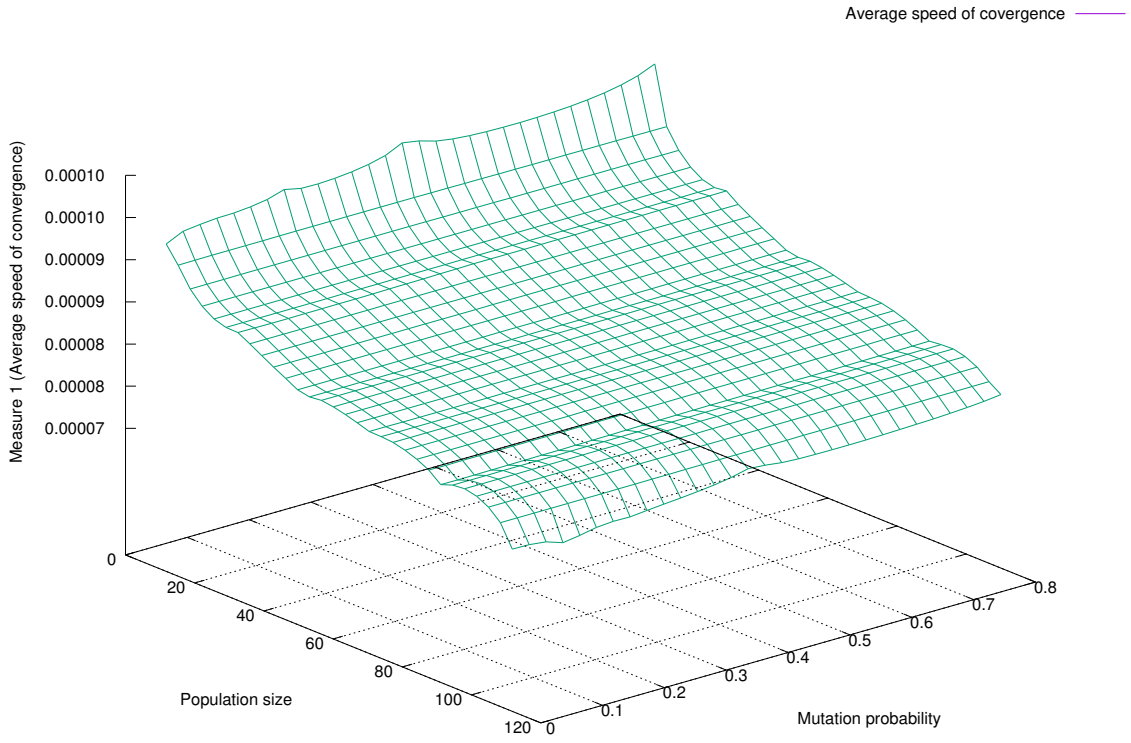

Figure 5: Surface of measure for first part of graph

Grain orientation

After selecting best configuration we performed many hundreds of run in order to get reliable results of GA.

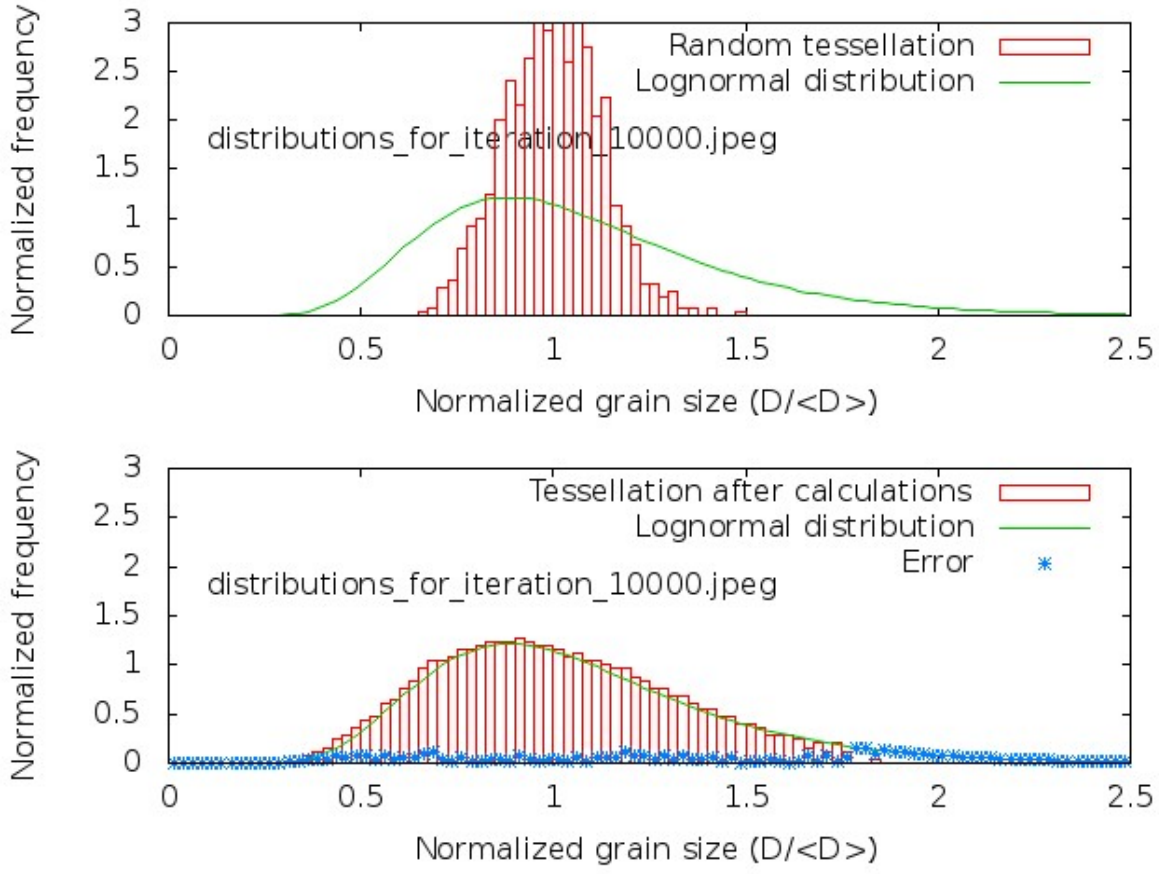

Figure 6: Best configuration result

Grain orientation

The same GA was used for achieving grain orientation distribution. But goal function was a partially defined Mackenzie function. This function describes distribution of so called misorientation angle. This angle is calculated in different way for different lattice types. But we consider only cubic lattices. For this GA also optimization of configuration is made.

Methodology

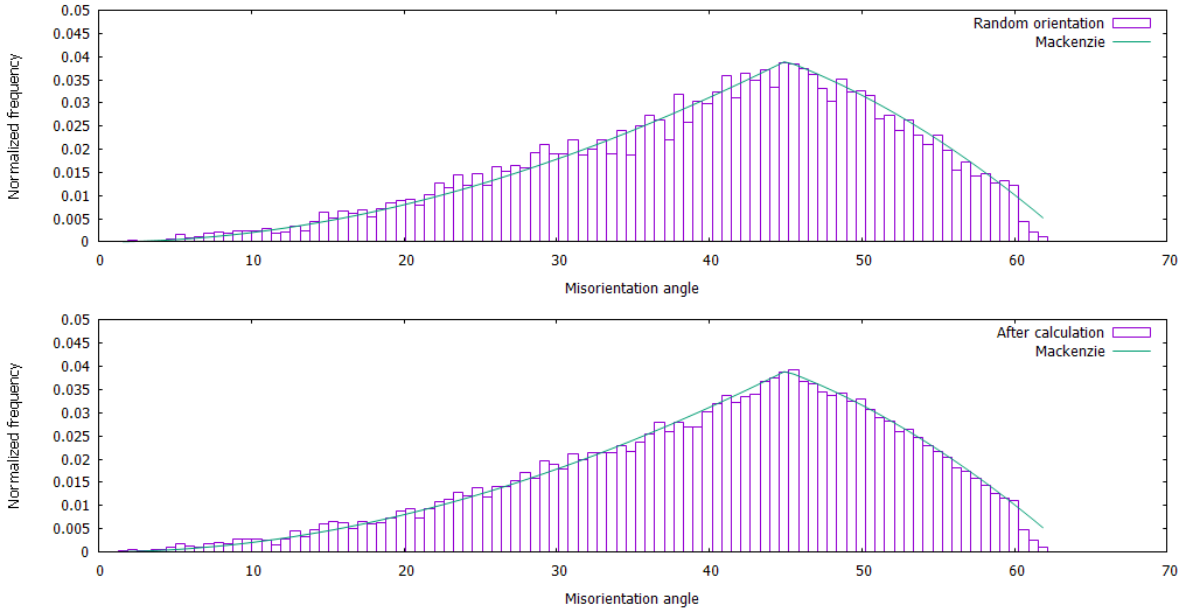

Figure 7: Best configuration result

Generation of atoms

After obtaining container with boundaries of potential grains inside it we have to fill this container with atoms. This procedure is made in way that firstly I generate atom structure that is twice more than diameter of the grain. It is needed to cover all possible rotation of atoms. Then I rotate atoms according to the Euler angles that I obtained in grain orientation distribution step. After I cut all excess atoms that go outside of grain.

Relaxation of structure

Relaxation means minimum energy of the system. After following three steps: GA for grain size distribution, GA for grain orientation distribution and atom generation we need to modify atomic structure in order to obtain stable system. This achieved by two steps: shifting generated lattices and removing of excess atoms. Shifting process is based again on GA. The same procedure is done for this GA as it was for previous cases.

Removing excess atoms is done based on calculating total energy and removing close to each other atoms and then recalculating total energy. If we obtain energy reduction then we accept this atom removing. We repeat this procedure till reaching expected energy level.

The last step is just running structure in LAMMPS with the same potential what we used for total energy calculation to check if structure is stable.

Conclusion

The aim of implementation of generalized procedure of realistic polycrystalline structure generation is achieved in this work. In fact we got useful tool for polycrystall generation according to the given distributions. In this case we are able to learn how this structure behaves and what physical parameters it has and this parameters will correspond to the expected experimental data.

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