

GPUQT: Graphics Processing Units Genetic Algorithm

Reference Manual

Version 1.0

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Chapter 1

Introduction

1.1 What is GPUGA?

GPUGA stands for Graphics Processing Units Genetic Algorithm. It is an efficient empirical potential fitting code using the genetic algorithm (GA) implemented on the graphics processing units (GPU). The implementation language is CUDA C++. It is developed for this paper [Fan et al. \(2019\)](#):

Zheyong Fan, Yanzhou Wang, Xiaokun Gu, Ping Qian, Yanjing Su, Tapio Ala-Nissila, A minimal Tersoff potential for diamond silicon with improved descriptions of elastic and phonon transport properties, <https://arxiv.org/abs/1909.11474>

If you use GPUGA in your published work, we kindly ask you to cite Ref. [Fan et al. \(2019\)](#).

This is version 1.0, and it can only fit the minimal Tersoff potential as proposed in Ref. [Fan et al. \(2019\)](#). We aim to implement more empirical potentials for version 2.0.

1.2 Feedbacks

You can email Dr. Zheyong Fan if you find errors in the manual or bugs in the source code, or have any suggestions/questions about the manual and code. The following email address can be used:

- [brucenju\(at\)gmail.com](mailto:brucenju(at)gmail.com)

1.3 Acknowledgments

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Chapter 2

Theoretical formalisms

See the above paper.

Chapter 3

Using GPUGA

The code has only been tested in linux operating systems and we assume that the user is using a linux operating system to compile and run this code.

3.1 Compile the code and run the examples

3.1.1 Compiling

After downloading and unpacking GPUGA, one can see three folders: `src`, `doc`, `tools`, and `examples`. The folder `src` contains all the source files. The folder `examples` contains all the examples. The folder `tools` contains a Matlab script for plotting Fig. 3 in the above paper. The folder `doc` contains the pdf file you are reading and the source files generating it.

To compile the code, first go to the `src` folder. The just type

```
make -f makefile.cpu
```

in the command line. This will produce an executable called `gpuga` in the `src` folder. The second line of `makefile` reads

```
CFLAGS = -std=c++11 -O3 -arch=sm_50 --use_fast_math
```

Change `gpuga` to the appropriate “compute capability” of your GPU. The minimum compute capability supported by GPUGA is 3.5.

3.1.2 Running

Go to the directory where you can see the `src` folder and type

```
src/gpuga < examples/input.txt
```

This will run the prepared example. To run your own calculations, just replace folder name (including absolute or relative path but excluding a “/”) as specified in `examples/input.txt` to your own working directory. Then you need to prepare some input files in the working directory, as describe below.

3.2 Input files for GPUGA

To run on simulation with GPUGA, you need to prepare three files in your chosen working directory: `ga.in`, `potential.in`, and `train.in`. We describe them below.

3.2.1 The ga.in input file

This file contains the controlling parameters defining the GA simulation. In this input file, blank lines and lines started with # are ignored. Each non-empty line starts with a keyword followed by one parameter. The valid keywords and their parameters are listed below.

1. **maximum_generation**

This keyword needs one parameter, which is the maximum number of generations in the GA evolution. It can be any positive integer. The default value is 1000.

2. **population_size**

This keyword needs one parameter, which is the population size (number of individuals in one generation). It can be no less than 20 and should be a multiple of 10. The default value is 200.

3. **parent_number**

This keyword needs one parameter, which is the number of parents in one generation. It can be no less than 10 and should be a multiple of 10. The default value is 100.

4. **mutation_rate**

This keyword needs one parameter, which is the initial mutation rate in GA evolution. It should be in $[0, 1]$. The default value is 0.2. The mutation rate will linearly decrease and reach 0 up to the **maximum_generation**.

3.2.2 The potential.in input file

This file contains information about the potential to be fitted. It has a fixed format. For example, the file `examples/si_diamond/potential.in` reads:

```
potential_type 1
cutoff         3.0
weight_force   0.05
weight_energy  0.15
weight_stress  0.8
D0             2.9 3.3
a              1.3 1.5
r0             2.2 2.4
S              2 2
n              0.5 0.8
beta           0 0.4
h              -0.8 -0.6
R1             2.8 2.8
R2             3.2 3.2
```

At each line, there is one character string and one or two numbers. To do new experiments, just keep the strings unchanged and modify the numbers. Here are some explanations:

- line 1: The type of the potential to be fitted, which can only be 1 (means the minimum Tersoff potential) in this version.

- line 2: The cutoff distance used for building the neighbor list for each configuration (see below), which should be a positive number.
- lines 3-5: The weighting factors for force, energy, and stress. They should be non-negative numbers. It is good to make their summation to be 1, although the code does not complain if this is not the case.
- lines 6-14: The lower (the first number in each line) and upper (the second number in each line) bounds of the potential parameters for the minimal Tersoff potential. The order of the parameters are the same as those in Table II of Ref. [Fan et al. \(2019\)](#).

3.2.3 The train.in input file

3.3 Output files of GPUGA

For each simulation, four output files will be generated in the working directory: `ga.out`, `force.out`, `energy.out`, and `virial.out`.

3.3.1 The ga.out file

3.3.2 The force.out file

3.3.3 The energy.out file

3.3.4 The virial.out file

Bibliography

Zheyong Fan, Yanzhou Wang, Xiaokun Gu, Ping Qian, Yanjing Su, and Tapio Ala-Nissila.
A minimal Tersoff potential for diamond silicon with improved descriptions of elastic
and phonon transport properties. *arXiv preprint arXiv:1909.11474*, 2019. URL <https://arxiv.org/abs/1909.11474>.