

User Manual

1. Introduction

MrBayes tgMC³ (version 1.1), a tight GPU implementation of MrBayes MC³, is a modified version of [MrBayes \(version 3.2\)](#) that enables accelerating Metropolis Coupled Markov Chain Monte Carlo (MC³) sampling on CUDA-compatible Graphics Processing Units (GPUs). MrBayes tgMC³ has not been designed to perform all features and settings that MrBayes has, it specifies a GTR + I and GTR + I + Γ model (a General Time Reversible model with a proportion of invariable sites and a gamma shaped distribution of rates across sites) for nucleotide sequences, which has the settings as

```
nucmodel = 4by4;  
nst = 6;  
rates = gamma or invgamma;  
datatype = dna;
```

The implementation of MrBayes tgMC³ needs at least one CUDA-compatible GPU card. In addition, two software packages are required to be installed before the running, which are CUDA toolkit and GPU computing SDK. The release version can be downloaded from [here](#) (CUDA 4.2 for Linux).

2. Compile and implement MrBayes tgMC³

2.1 Prerequisites

Before using multiple CPU processes, the value of CUDA variable in the make file should be changed to **YES**. Make sure import `CUDA_INSTALL_PATH` and `SDK_INSTALL_PATH` to environment variable list before issuing **make** command, otherwise, the OS may not find the correct compiler, CUDA-related libraries and head files. Type command **set** will display environment variable list in terminal.

Currently, MrBayes tgMC³ is implemented on a machine with one core and one GPU.

2.2 Installation of MrBayes tgMC³

Provided that the prerequisites have been met, MrBayes tgMC³ is ready to be installed.

Step1: Download the source code of MrBayes tgMC³. MrBayes tgMC³ for Linux is available from:

https://github.com/s0897918/gpu_mrbayes_32

and the name of the package is:

gpu_mrbayes_32.tar

Step2: Unzip the package and compile it as:

```
tar -xvf gpu_mrbayes_32.tar  
cd gpu_mrbayes_32/src  
make clean  
make
```

2.3 Implement MrBayes tgMC³

Let DATA denote the name of the input data file, the immediate command

```
./mb DATA
```

results in running MrBayes tgMC³ by one CPU process. For example,

```
./mb dataset1(26x1546).nex
```

The file dataset1(26x1546).nex is one of the datasets used to benchmark MrBayes tgMC³, which has been included in the downloadable MrBayes tgMC³ package.

MrBayes tgMC³ has been tested on GTX480 and GTX580. However, it may have problems when executed on other GPU platforms. If there are any bugs for MrBayes tgMC³, please do not hesitate to contact the author. s0897918@gmail.com