

# GPU-oriented MrBayes Using Vertical Partitioning

## User Manual

### 1. Introduction

MrBayes tgMC<sup>3</sup> (version 2.0), GPU-oriented MrBayes Using Vertical partitioning, is a modified version based on [MrBayes \(version 3.1.2\)](#) and [MrBayes tgMC<sup>3</sup> \(version 1.0\)](#). It enables accelerating Metropolis Coupled Markov Chain Monte Carlo (MC<sup>3</sup>) sampling on CUDA-compatible Graphics Processing Units (GPUs). MrBayes tgMC<sup>3</sup> has not been designed to perform all features and settings that MrBayes has, it specifies GTR/HKY85/F81/JC69 models for nucleotide sequences with a user defined number of gamma category to simulate the rate variation among sites. A commonly used setting is as:

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

Which specifies a General Time Reversible (GTR) model with a proportion of invariable sites and a gamma shaped distribution of rates across sites (4 gamma categories).

The implementation of MrBayes tgMC<sup>3</sup> needs at least one CUDA-compatible GPU card. In addition, two software packages are required to be installed before using the software, which are CUDA toolkit and GPU computing SDK. The release version can be downloaded from [here](#) (CUDA 6.5 for Linux).

### 2. Compile and implement MrBayes tgMC<sup>3</sup>

#### 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.

#### 2.2 Installation of MrBayes tgMC<sup>3</sup>

Provided that the prerequisites have been met, MrBayes tgMC<sup>3</sup> is ready to be installed.

Step1: Download the source code of MrBayes tgMC<sup>3</sup>. MrBayes tgMC<sup>3</sup> for Linux is available from:

[https://github.com/s0897918/MrBayes\\_tgMC\\_2.0/](https://github.com/s0897918/MrBayes_tgMC_2.0/)

and the name of the package is:

**tg\_mrbayes\_v2.0.tar**

Step2: Unzip the package:

**tar -xvf tg\_mrbayes\_v2.0**

Step3: choose the suitable package:

There are two packages, namely gamma4\_specified and general. The former is optimized for the analysis with a fixed number of gamma categories, i.e. 4. The latter can be used under a more general definition of the number of gamma category. However, gamma4\_specified is better to be used when you use 4 gamma categories, as it runs faster using CUDA.

Step 4: compile the source code, e.g. using the gamma4\_specified one:

**cd tg\_mrbayes\_v2.0/gamma4\_specified**  
**make clean**  
**make**

### 2.3 Implement MrBayes tgMC<sup>3</sup> on a single GPU

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

**./mb DATA**

results in running MrBayes tgMC<sup>3</sup> by one CPU process.

### 2.4 Implement MrBayes tgMC<sup>3</sup> on multiple GPUs

Make sure that the MPI flag in Makefile is set to YES, the immediate command:

**mpiexec -n 2 ./mb dataset1(26x1546).nex**

results in running MrBayes tgMC<sup>3</sup> by two CPU process with each process having one GPU card.

MrBayes tgMC<sup>3</sup> (v2.0) was tested on GTX580, GTX680 and Tesla K40. However, it may have problems when executed on other GPU platforms. If there are any bugs for MrBayes tgMC<sup>3</sup>, please do not hesitate to contact the author:

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