

MrBayes goMC³ (version 1.0) User Manual

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1. Introduction

MrBayes goMC³: optimizing the Bayesian inference of phylogeny, is a modified version of [MrBayes \(version 3.1.2\)](#) that enables accelerating Metropolis Coupled Markov Chain Monte Carlo (MC³) sampling on CUDA-compatible Graphics Processing Units (GPUs). MrBayes goMC³ is not designed to perform all features and settings that MrBayes has, it specifies a commonly used GTR + I + Γ model (a General Time Reversible model with a proportion of invariable sites and 4 gamma shaped distribution of rates across sites) for nucleotide sequences, which has the settings as

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

The implementation of MrBayes goMC³ 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 goMC³

2.1 Prerequisites

MrBayes goMC³ supports concurrent execution of multiple CPU processes by using Message Passing Interface MPICH2 (version 1.1 or above). Before using multiple CPU processes, the value of MPI variable in Makefile 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.

By default, we assume that MrBayes goMC³ is implemented on a machine with one core and one GPUs, and the maximum number of GPU can be set in cuda.cu file. The number of CPU process should be equal to the number of GPU in use.

2.2 Installation of MrBayes goMC³

Provided that the prerequisites have been met, MrBayes goMC³ is ready to be installed.

Step1: Download the source code of MrBayes goMC³. MrBayes goMC³ for Linux is available from https://github.com/s0897918/MrBayes_goMC3,

The package name for installation is *go_mrbayes.tar*

The package name for dataset is *dataset.rar*

The package name for user manual is *User manual.pdf*

Step2: Unzip the source package and compile it as:

```
untar -xvf go_mrbayes.tar
cd go_mrbayes/goMC^3
make clean
make
```

2.3 Implement MrBayes goMC³

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

```
./mb DATA
```

results in running MrBayes goMC³ by only one CPU process. For example,

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

For using multiple CPU processes, the command below will be initiated

```
mpiexec -n <p> ./mb DATA
```

Where <p> denotes the number of concurrent CPU processes (which should be no more than the number of CPU cores), for example,

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

The file dataset1(26x1546).nex is one of the datasets used to benchmark MrBayes goMC³, which has been included in the downloadable MrBayes goMC³ package.

MrBayes goMC³ has been tested on GTX480 (CUDA), Tesla C2075 (Feimi) and GTX680 (kepler). However, it may have problems when executed on other GPU platforms. If there are any bugs for MrBayes goMC³, please do not hesitate to contact the author. s0897918@gmail.com