MrBayes tgMC^3 (version 1.1) User Manual

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1. Introduction

MrBayes tgMC^3 (version 1.1), a tight GPU implementation of MrBayes MC^3, is a modified version of MrBayes (version 3.2) that enables accelerating Metropolis Coupled Markov Chain Monte Carlo (MC^3) sampling on CUDA-compatible Graphics Processing Units (GPUs). MrBayes tgMC^3 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 tgMC^3 needs at least one CUDA-compatible GPU card. In addition, two software packages are required to been 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 tgMC^3

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 tgMC^3 is implemented on a machine with one core and one GPU.

2.2 Installation of MrBayes tgMC^3

Provided that the prerequisites have been met, MrBayes tgMC^3 is ready to be installed.

Step1: Download the source code of MrBayes tgMC^3. MrBayes tgMC^3 for Linux is available from:

https://github.com/s0897918/cuda-mrbayes/

and the name of the package is:

tg_mrbayes_v1.1.tar

Step2: Unzip the package and compile it as:

tar -xvf tg_mrbayes_ v1.1.tar
cd tg_mrbayes _v1.1/src
make clean
make

2.3 Implement MrBayes tgMC^3
Let DATA denote the name of the input data file, the immediate command

./mb DATA

results in running MrBayes tgMC^3 by one CPU process. For example,

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

The file dataset1(26x1546).nex is one of the datasets used to benchmark MrBayes tgMC^3 , which has been included in the downloadable MrBayes tgMC^3 package.

MrBayes tgMC^3 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 tgMC^3, please do not hesitate to contact us. s0897918@126.com