

QuickProbs 2: User's Manual

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Usage

QuickProbs 2 is a fast and accurate algorithm for multiple sequence alignment suited for massively parallel architectures (compatible with OpenCL). It is provided with two binaries for CPU and OpenCL devices (like GPU). All parameters suitable for the CPU version are also supported by the OpenCL binary. The latter additionally requires an OpenCL platform and device to be specified. Below one can find typical QuickProbs 2 use cases.

`quickprobs-2.05`

Displays the detailed information about QuickProbs 2 options.

`quickprobs-cl-2.05`

Displays the detailed information about QuickProbs 2 options and available OpenCL devices.

`quickprobs-2.05 input`

Aligns sequences from *input* file and prints the result on the standard output (other messages are by default printed on the standard error stream). Both input sequences and output alignment are in the FASTA format. The calculations are performed on a central processor (without OpenCL) and distributed among all detected cores.

`quickprobs-2.05 input -o output`

Aligns sequences from *input* and stores the result in *output* file.

`quickprobs-2.05 input -o output -v`

Runs algorithm in a verbose mode (prints a lot of debug information).

`quickprobs-2.05 input -o output -t 6`

Distributes computations on 6 CPU threads.

`quickprobs-cl-2.05 input -o output -p 0 -d 1`

Runs QuickProbs in OpenCL mode on device 1 from platform 0. Use this option to perform the calculations on massively parallel devices like graphics processors. Note, that central processors are also OpenCL devices. Nevertheless, OpenCL code in QuickProbs 2 was especially optimised for GPUs architectures and was not tested on CPUs! It is suggested to use the CPU binary to perform analysis on a central processor only.

`quickprobs-2.05 input -o output -n`
Runs the algorithm in a nucleotide mode.

`quickprobs-2.05 input -o output -c 3`
Runs the algorithm using 3 consistency transformations (default: 2 for number of sequences < 50, 1 otherwise).

`quickprobs-2.05 input -o output -r 3`
Runs the algorithm using 60 refinement iterations (default: 30 for number of sequences < 50, 100 otherwise).

`quickprobs-2.05 input -o output --mem-limit 30000`
Attempts to fit computations into 30,000 MB of RAM memory (default: 55,000 MB).

Bulk mode

For convenience QuickProbs 2 has been equipped with bulk mode which allows multiple sequence sets to be processed at a single run. In bulk mode *input* and *output* parameters have to be existing directories. Software automatically process all files from *input* and stores alignments in *output* under same file names.

OpenCL configuration

GPU driver timeout under Windows

By default Windows resets GPU driver after 2 seconds of non-responsiveness. This may be insufficient for QuickProbs. To change this setting do the following:

1. Go to registry editor: Start → Run → Type in "regedit".
2. Go to "HKEY_LOCAL_MACHINE \SYSTEM \CurrentControlSet \Control \GraphicsDrivers".
3. Create a key of type "DWORD (32-bit)" and name "TdrDelay" with a value of 10 as Decimal value.

AMD graphics cards

In order to maximally utilise computational power of AMD graphics processors some environment variables have to be set. They are described below.

1. `GPU_MAX_WORKGROUP_SIZE` For unknown reasons maximum size of workgroup for AMD devices reported by OpenCL is lower than physical hardware limit. E.g. for Radeon 7970 it reports maximum size of 256 while real limit is 1024. This environment variable allows one to override the default setting. Read in the device documentation maximum physical size of workgroup and set the variable to this value.

2. `GPU_MAX_ALLOC_PERCENT` This value indicate maximum percentage size of single OpenCL buffer related to the total size of GPU global memory.

NVidia graphics cards

Some instabilities were experienced when running OpenCL on GeForce 980 under Windows 10 x64. In particular, from time to time the software crashed during OpenCL initialisation. Most probably this was due to bug in 359.06 driver—the same situation was observed for other OpenCL applications. If you encounter similar problem, please run QuickProbs 2 again.