AMD **Accelerated** Parallel Processing
TECHNOLOGY

SAMPLE

MD

1 Overview

1.1 Location

`$<APPSDKSamplesInstallPath>\samples\C++Amp\`

1.2 How to Run

See the *Getting Started* guide for how to build samples. You first must compile the sample.

Use the command line to change to the directory where the executable is located. The default executables are placed in `$<APPSDKSamplesInstallPath>\samples\C++Amp\bin\x86\` for 32-bit builds, and `$<APPSDKSamplesInstallPath>\samples\C++Amp\bin\x86_64\` for 64-bit builds.

Type the following command(s).

1. `MD`

   This runs the program with the default options `-i 10`.

2. `MD -h`

   This prints the help file.

Ensure Microsoft® Visual Studio® 2012 or higher is installed.

1.3 Command Line Options

Table 1 lists, and briefly describes, the command line options.

Table 1 Command Line Options

Short Form	Long Form	Description
`-h`	`--help`	Show all command options and their respective meaning.
`-q`	`--quiet`	Quiet mode. Suppresses text output.
`-e`	`--verify`	Verify results against reference implementation.
`-t`	`--timing`	Print timing.
`-d`	`--deviceId`	Select deviceId to be used (0 to N-1, where N is the ID of the device to be used).
`-v`	`--version`	AMD APP SDK version string.
`-i`	`--iterations`	Number of times to repeat each algorithm.

2 Introduction

This is a sample which can be used to measure the force putting on the point from others by using C++ AMP. First it uses a mathematically simple model called Lennard-Jones equation to approximate the interaction potential between a pair of neutral points. The equation of the L-J potential is:

$$V_{LJ} = 4\varepsilon[(\frac{\sigma}{r})^{12} - (\frac{\sigma}{r})^{6}]$$

Where ε is the depth of the potential well, σ is the finite distance at when the inter-potential is zero, r is the distance between the particles.

Then we can get the force coefficient from the ratio of potential and distance square. The force equate to the force coefficient multiplied by the distance.

Here, we only consider interactions within the cut-off distance (default is 4.0).

3 Implementation Details

1. The Lennard-Jones potential is a mathematically model for approximating the interaction potential between a pair of neutral points. The equation of the L-J potential is

   $$V_{LJ} = 4\varepsilon[(\frac{\sigma}{r})^{12} - (\frac{\sigma}{r})^{6}]$$

   For the performance, the equation has been simplified to:

   $$V_{LJ} = \frac{1}{r^6}[4\varepsilon\sigma^{12}\frac{1}{r^6} - 4\varepsilon\sigma^{6}]$$

   The simpler form is:

   $$V_{LJ} = \frac{1}{r^6}[C_1\frac{1}{r^6} - C_2]$$

   Where C_1 is $4\varepsilon\sigma^{12}$, which we set it to 1.5, and C_2 is $4\varepsilon\sigma^{6}$ which we set it to 2.0 in this sample. The C_1 and C_2 are constant values.
2. Then we can get the relationship about the force and the distance between a pair of neutral points. It is equal to the ratio of VLJ and distance square. The equation is:

   $$F_{LJ} = \frac{V_{LJ}}{r^2}$$

   The force between the two points is the result of multiplying FLJ and distance.
3. Adding the each forces from other points to this one, we can get the total force on the point.

   Here, we only consider 64 closest interactions within the cut-off distance (default is 4.0).

4 References

1. Lennard-Jones, J. E. (1924), "On the Determination of Molecular Fields", Proc. R. Soc. Lond. A 106 (738): 463–477

Contact

Advanced Micro Devices, Inc.
One AMD Place
P.O. Box 3453
Sunnyvale, CA, 94088-3453
Phone: +1.408.749.4000

For AMD Accelerated Parallel Processing:

URL: developer.amd.com/appsdk
Developing: developer.amd.com/
Forum: developer.amd.com/openclforum

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