

HACCmk

Summary Version

1.0

Purpose of Benchmark

The Hardware Accelerated Cosmology Code (HACC) framework uses N-body techniques to simulate the formation of structure in collisionless fluids under the influence of gravity in an expanding universe. The main scientific goal is to simulate the evolution of the Universe from its early times to today and to advance our understanding of dark energy and dark matter, the two components that make up 95% of our Universe. HACCmk is the kernel routine of the code which calculates the short force evaluation with an N^2 algorithm.

Characteristics of Benchmark

The short force evaluation kernel is compute intensive with regular stride one memory accesses. It is looping over a predefined list of particles and their neighborhoods and calculates the force values for each particle. The force evaluation for each particle can be independently evaluated, the current implementation is using OpenMP “parallel for” pragma statement to parallelize over the loop of particles. The calculation of the force for each particle is implemented as a separate function with particle coordinates, their mass, the list of coordinates of neighborhood particles, and their masses, as the input arguments. The force is approximated with a power function over the distance between particles and a 5-th order polynomial in the remainder.

Mechanics of Building Benchmark

The compile options are specified in correspondent Makefile. CFLAGS_KERNEL variable should include aggressive optimization options without recognition of OpenMP directives. CFLAGS_MAIN variable should specify the least aggressive set of optimization options to prevent optimization of the timing statement in the main program. This variable must include the option that recognizes OpenMP directives. The timing routine should be changed to the one appropriate for a platform. This benchmark uses a low level CPU clock accurate resolution timer long long int timebase(). Conversion from CPU cycles to seconds is performed with the help of a conversion coefficient "MHz", defined in main.c:16. Alternative portable timing routine, based on gettimeofday() function call, is also provided in the mysecond.c file.

Mechanics of Running Benchmark

Submission scripts are written for Cobalt scheduler - the standard utility used in Argonne Leadership Computing Facility; however, they can be modified accordingly to a preferred scheduler on the system. The program is not using any arguments. Upon submission of the job, the number of threads should be specified with standard OMP_NUM_THREADS env. variable. The benchmark reports the number of used OpenMP threads, the computation run time, the result of the computation, as well as self verification of the results. The typical output for a Blue Gene/Q node was obtained with the provided CheckAll script. Similar results are expected upon response.

```
Number of OMP threads 1
Kernel elapsed time, s: 210.85903916
Total elapsed time, s: 211.04163578
```

Result validation: 6636045675.12190628
Result expected : 6636045675.12190628

Number of OMP threads 2
Kernel elapsed time, s: 105.41948631
Total elapsed time, s: 105.60241941
Result validation: 6636045675.12190628
Result expected : 6636045675.12190628

Number of OMP threads 4
Kernel elapsed time, s: 53.13009598
Total elapsed time, s: 53.31305897
Result validation: 6636045675.12190628
Result expected : 6636045675.12190628

Number of OMP threads 8
Kernel elapsed time, s: 26.69305273
Total elapsed time, s: 26.87610440
Result validation: 6636045675.12190628
Result expected : 6636045675.12190628

Number of OMP threads 16
Kernel elapsed time, s: 13.76628785
Total elapsed time, s: 13.94928015
Result validation: 6636045675.12190628
Result expected : 6636045675.12190628

Number of OMP threads 32
Kernel elapsed time, s: 9.46185759
Total elapsed time, s: 9.64484288
Result validation: 6636045675.12190628
Result expected : 6636045675.12190628

Number of OMP threads 64
Kernel elapsed time, s: 7.36997379
Total elapsed time, s: 7.55316004
Result validation: 6636045675.12190628
Result expected : 6636045675.12190628

Verification of Results

The benchmarks reports the expectation value as well as the computed values for the aggregate force over all particles.