SSE/AVX and GPU2 with NBODY6

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We provide some notes on the use of the SSE (Streaming SIMD Extension), AVX (Advanced Vector eXtension) and GPU (Graphics Processing Unit) versions for running `NBODY6`, first developed at the Institute of Astronomy in April 2008. As before, the standard code is compiled by typing `make nbody6` in the directory `Ncode` and there are no new routines inside the `Makefile`. For the GPU2 version, type `make gpu` in dir `GPU2`.

Hardware requirements for the SSE/AVX/GPU versions are either a multi-core CPU of the type x86 or x86_64 processors with SSE/AVX support and/or a GPU with CUDA support. Core i5/i7 with 64-bit OS is recommended for high performance calculations with AVX. GeForce GTX 660Ti or GTX 680 is adequate for a single GPU.

Software requirement: AVX requires support of both the compiler and kernel. For simplicity, we mention that combination of CentOS 6.x and CUDA 4.x or later can compile and execute the code successfully.

The directory `GPU2` has several extra Fortran routines which contain the new procedures, as well as some modified standard routines. The subdirectory `lib` holds the GPU library for regular force. To obtain the GPU2 version `nbody6.gpu`, type `make gpu` in the directory `GPU2` while `make avx` produces `nbody6.avx`. In both versions we use the OpenMP directives in some routines. The executable is sent to the run subdirectory `GPU2/run` which also contains simple input templates (or see dir `Docs`). Input for different simulations remains as before, with most options having the usual meaning.

Users can specify the number of threads per process by setting the environment variable `OMP_NUM_THREADS`. Since we use multiple cores, the CPU time in the output is larger than the wall-clock time in the ADJUST line. The actual time for data send and gravity calculation is given on the screen at the end, together with the corresponding Gflops.

Some comments on extra routines in dir GPU2 or `lib`.

gpunb.velocity.cu: main routine for GPU library in CUDA (dir `lib`).

intgrt.omp.f: integration flow control for GPU or SSE (also parallelized).

repair.f: modification of array LISTQ after new or terminated KS.

jpred.f: standard prediction of X & XDOT and resolved KS components (J > N).

jpred2.f: neighbour prediction of single particle (local arrays).

ksres3.f: transformed coordinates and velocities of KS pairs (local arrays).

cxvpred.cpp: full X & XDOT prediction in C++ except for TPRED(J)=TIME.

gpucor.f: regular force corrector and irregular force loop.

cmfirr.f: irregular force on perturbed c.m.'s.

cmfirr2.f: irregular force on singles from c.m.'s at regular force times.

kspert.f: KS perturbation force loops done in C++ by cnbint.cpp.

nbintp.f: parallel irregular force corrector with fast neighbour force.

nbint.f: fast neighbour force (< NPMAX), corrector & decision-making.

cnbint.cpp: neighbour force loop (in C++ with SSE).

adjust.f: standard energy check routine but calls energy2.f.

gpupot.gpu.cu: fast evaluation of all potentials on GPU (in dir `lib`).

energy2.f: summation of individual potentials after differential correction.

phicor.f: differential potential corrections due to binary interactions.

swap.f: randomized particle swapping at T = 0 (reduces crowding).

Optimization:

Optimized performance is achieved by minimizing the number of overflows which results in the last block members (< NIMAX) being recalculated. However, small average neighbour numbers (also in #9 output line) may affect the accuracy. Based on preliminary tests, a relatively large value of NNBMAX and option #40 = 2 (or 3 for decreasing NNBMAX after escape) appears to be a good strategy. The fast routine cnbint.cpp is used by gpucor.f, nbint.f, nbintp.f and kspert.f. Note that all arguments are offset by -1 in cnbint.cpp for consistency with the C++ convention. Later we included NBMAX in common6.h and updated it in adjust.f as MIN(NNBMAX+150,LMAX-5). This is now used as a practical upper limit by GPUNB_REGF which reduces overflows (various conditions involving NNBMAX in gpucor.f have been removed).

Options:

In order to save time on the host (large N only), #38 = 2 restricts the neighbour force derivative corrections to 1 % regular force change, while for #38 = 1 all corrections are done. The CPU time may also be reduced by saving the common blocks on fort.1 only at every main output as a backup for rare restarts (#1 = 2 and #2 = 0). Option #40 >= 2 stabilizes the average neighbour number (in adjust.f) on a fraction of the maximum (e.g. NNBMAX/5) for small overflow numbers. The overflow counters (#9 OVERFLOWS; current and accumulated) at main output provide useful diagnostics of the behaviour (#33 >= 2). To be consistent with decreasing particle numbers, the maximum membership is reduced by a square root relation scaled by the initial value (#40 = 3).

GPUIRR

The new irregular library deals with prediction of active particles and evaluation of neighbour forces. In the case of no regular force calculation, the predictions are done by GPUIRR_PRED_ACT or PRED_ALL. Here the parameter NPACT, defined in intgrt.omp.f, is used to decide between the two versions of prediction, respectively. Irregular forces for active particles are obtained by the SSE vector procedure GPUIRR_FIRR_VEC. Finally corrected quantities are sent to this library by GPUIRR_SET_JP at the end of the cycle.