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Parallel Computing with NBODY6++
with and without GPU

Thursday, March 4, 2021, Uni Heidelberg, GPU Block Course

1. Compiling and Running NBODY6++

1.1 Compiling and running the code on kepler

```
tar xvfz worknb6.tgz
cd worknb6
module purge
module load cuda
make clean ; make -j mpich
ls -ltr
```

You find the executable file nbody6.mpi, move it to Run/nbody6.mpi :

```
mv -i nbody6.mpi Run/

make clean ; make -j mpichgpu_kepler
ls -ltr
```

You should find the executable file nbody6.gpu

```
mv -i nbody6.gpu Run/

cd Run/
ls -lrt
```

Here is the batch job script mpi_script.sh and gpu_script.sh . You should run it with nbody6.mpi for nodes=1,2,4,6 (gres=gpu:0) and with nbody6.gpu for nodes=1,2,4,6 (gres=gpu:1). Always use the student queues #SBATCH -p Student_CPU and Student_GPU .

The standard job prepared for you uses 5000 particles, and simulation time of 5 model units (check output how many years). The input file containing some control data is in5000.comment.

You can change the particle number, either by using another input file (like in10k.comment or in32k.comment), or change N directly in the input file. For our course you will need outputs of 8 jobs (mpi and gpu, 1,2,4,6 nodes), 5000 particles. Using more particles is also ok, but be considerate to all of us, the runs take some time, we have many runs, and the machine will be full.

Additional voluntary study (not required):

The files like in10k.ktg.sev switch on astrophysics. This will include astrophysical stellar evolution and produce data for a Hertzsprung Russell diagram (HRD, temperature/luminosity) in sev.83. In this file you get lines with following columns:

time, index, name, stellar type, pos. in cluster, mass, log luminosity , log radius, log effective temperature (last three in solar units).

Astronomers like to plot log(luminosity) as a function of effective temperature (high T left, low T right on the x-axis), that is called an HRD.

The code also produces a lot of other output files. Most of them are not interesting for us. We will look mainly at the output listing such as e.g. out5000.xxx.nnnnn ... Here xxx is gpu or mpi, and nnnnn is a job id number.

```
grep ADJUST out5000...xxx.nnnnn
```

You can see whether the run has done well. To extract the timing data relevant for the course exercise, find the lines below ADJUST, headed by “PE N ttot...” .

2 Parallel Communication Schemes and Literature

NBODY6++ runs in the SPMD (Single Program Multiple Data) Scheme. It means when you start the parallel NBODY6++ run on n nodes (by using the command mpirun -np n …), n identical copies of the program will start. In parallel sections these copies of the code share their work and communicate data with each other through a software package called MPI (message passing interface). Every node is using its GPU.

NBODY6++ uses for communication a copy algorithm (all new information is copied immediately to all nodes); other algorithms are ring algorithm or (hyper)systolic algorithm, see Dorband, Hemsendorf, Merritt, 2003 (Journ. Comp. Phys.); Makino (2002). If the number of particles per node is large enough, all algorithms scale equally well. The copy algorithm in NBODY6++ is implemented manually with `MPI_SENDRECV`. Current modern implementations of `MPI_ALLREDUCE` will be equally efficient.

3 Hands-On Experiment on parallel computer

3.1 Profiling for NBODY6++

The code measures the wall clock time used for many things:

total, regular force, irregular force, adjust, regularised, prediction, overhead for parallelisation, communication time…

Your task: Do some experiment - run on 1,2,4,6... processors, with and without GPU usage, as explained above. Find, cut and paste the lines below the timing header (“PE   N ttot..”). Use the last one in your job (after ADJUST TIME= 5.00).

Explanation of times in output (line below 'PE   N'):

```
ttot: total  wallclock time
treg: regint, regular force (PAR)
tirr: nbint, neighbour force (PAR)
tadj: energy check (PAR)
tinit: computing of initial model (PAR)
tsub,tsub2: communication time using MPI_SENDRECV
xtsub1,xtsub2: number of bytes transferred
```

(PAR) means these routines are parallelised (contain shared work and MPI functions); there are more times listed, but we do not need them here. treg, tirr, tinit and tadj are required to determine X (see below); ttot, treg, tirr, tpred, and tcomm = tsub+tsub2 should be plotted as a function of number of nodes used (1,2,4,6), both for MPI and GPU jobs. What is the maximum speedup we get, without GPU, with GPU? What is the prediction of Amdahl's law? Note that the speed-up should be measured relative to the single node case;

3.2 Example Solution for NBODY6++ Tasks:

Here are my time measurements (taken from output files out.....):

```
 PE  N      ttot          treg     tirr     tpredtot  tint     tinit     tks     ttcomm   tadj    tmov     tprednb   tsub    tsub2   xtsub1   xtsub2
  1  5000   517.01170   447.73    43.23     0.00    504.89     4.20     0.22     0.00     7.83     1.46     6.85     0.00     0.00 0.00000D+00  0.00000D+00
  2  5000   273.74747   226.19    24.01     0.00    266.98     2.28     0.23     0.00     4.38     3.94     6.86     0.69     1.16 2.35923D+09  3.00958D+09
  4  5000   154.28701   110.07    14.23     0.00    150.33     1.29     0.24     0.00     2.56     8.72     6.82     1.72     2.39 3.53682D+09  4.51333D+09
  6  5000   110.29107    74.53     9.87     0.00    107.22     0.98     0.22     0.00     1.99     8.29     6.70     2.15     1.89 3.92945D+09  5.01460D+09
```

Calculate Amdahl's Law:

Let X be the part of my program (in terms of computing time) which can be parallelised. The sequential computing time Tseq is normalized to unity (1), and can be expressed as:

$T_{seq} = 1 = X + (1-X)$

The parallel computing time T_{par} under ideal conditions (ideal load balancing, ultrafast communication):

$T_{par} = X/p + (1-X)$ with number of nodes (number of GPUs) p

Then the speed-up of the program $S = T_{seq} / T_{par}$:

$S = 1 / (1-X+X/p)$

Note the limit if p is very large: S = 1/(1-X). We find from our measurements with NBODY6++ given above: X = (treg + tirr + tinit + tadj) / ttot = 503 / 517 = 0.97 .
Hence S = 1/(0.03 + 0.97/p), for large p max speed-up: S = 1/0.03 = 33.3333 (Note: this is only for 5000 Particles - for larger N we get MUCH higher X...) So, if we know X and p we can compute a predicted speedup S, and with that predict a parallel computing time by using

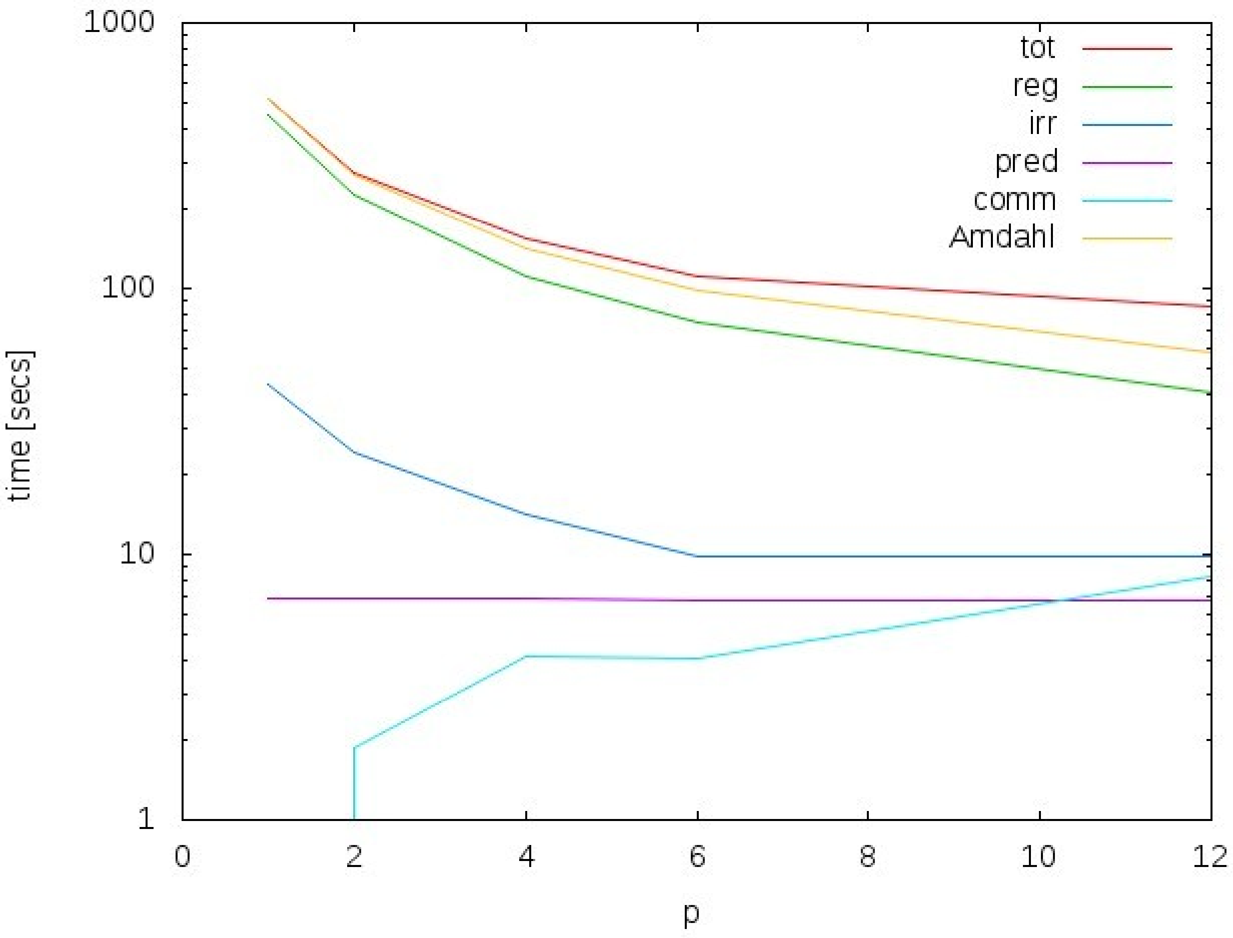
$T_{par,p} = T_{seq}/S$

The times $T_{par,p}$ are used to make the plotted line for Amdahl's law below..

Use gnuplot (for example):

```
set logscale y
plot 'time' u 1:3 w l t'tot', '' u 1:6 w l t 'reg', '' u 1:7 w l t'irr', \
                        '' u 1:($13+$14) w l t'comm', '' u 1:(517.*(0.03+0.97/$1)) w l lt 9 t'Amdahl'
```

See an example result below. Your results may deviate, look less nice, this is usually due to the high load of the kepler computer during the course. If you have successfully finished the 8 runs and collected your data, no matter whether they look good or bad, it is ok to pass the course.



Summary of your tasks to pass the course; please turn in the following results to your tutors:

1.) Two plots showing the times ttot, treg, tirr, tpred, and tcomm = tsub+tsub2 (communication time) as a function of p – one for MPI, one for GPU jobs. Plot also the predicted times obtained from Amdahl's law.
2.) A data file containing the data you have used for 1.); or a notice where we can find the file on kepler. **Please do not delete the output files of your 8 runs, because they are proof that you did the experiment.**
3.) A few (one, two, three...) sentences for interpretation: How good is Amdahl's law working? How good works GPU acceleration? Did you get outliers / bad results which do not match expectations? Anything else you like to mention. And please also questions if there are.