

Rainer Spurzem

Parallel Computing

1. Introduction to Scalability (Parallel Thinking)

Saturday, Nov. 22, 2014, KIAA, 11:00 a.m. - 12:30 p.m.

- The 1st lecture of Prof. Wen-mei Hwu will be partly presented (pp. 19-35) and discussed. See: http://silk0.bao.ac.cn/nb6mpi/lecture1_computational_thinking_Beijing_2012.pdf
- What is NBODY6++?
Parallel, GPU Accelerated Version of NBODY6
- Profiling, Performance Optimisation for NBODY6/6++
- Hands-On Experiment on parallel computer 老虎 at NAOC.

1.1 Introduction

- The 1st lecture of Prof. Wen-mei Hwu **(partly only!)**.

Parallel Thinking – Scalability, Data Parallelism, Work Parallelism

Memory Bandwidth, Amdahl's Law, Load Balance, Algorithm Complexity

If X is the fraction of a program's operations which can be parallelised, then the maximum speed-up S using a large number of parallel processors is $S = 1/(1-X)$. Examples: $X = 0.5$; $S = 2$.

$X = 0.99$; $S = 100$. Here we have used the assumption that the number of processors is large compared to unity. There are more precise formulae for Amdahl's law with finite number of processors.

1.2 Apply to NBODY6++

Memory Bandwidth/Amdahl's Law/Load Balance

Main Differences Between NBODY6 and NBODY6++:

- Parallel Work Structure (intgrt.F, Do-Loops)
- Contiguous Data Structure (intgrt.F, XMPI, YMPI)
- Control average neighbour number by NNBOPT
- Parallel KS-Integration/Parallel Prediction
- Input File: Parameters isernb, iserreg, iserks - serial execution if block size is smaller than isernb (for nbint) / iserreg (for regint) / iserks (for ksint)

Some useful but not so important differences:

- different filenames (comm.1, comm.2, conf.3, sev.82, bev.83, lagr.7, and so on)
- more output, better format (Lagrangian radii, etc)
- many more small differences (Makefile or configure, directory structure)

Usage of .F files:

intgrt.F is pre-processed with C-Preprocessor; it evaluates so-called preprocessor directives in the source code; they start with # , for example:

```
#ifdef PARALLEL
...
#endif
```

Preprocessor directives are selected with a compiler option:

-D PARALLEL compiles code between #ifdef PARALLEL and #endif.

Without -D PARALLEL these code lines will not be used!

WARNING - never keep .f if you have .F - the preprocessor directives will fail.

2. Introduction to Many-Core Programming (GPU's for Parallel Computing)

Saturday, Nov. 22, KIAA, 2:00 p.m.

- What is a GPU? Why it can be so fast?
- Simple CUDA Example
- Hands-on Experiments on 老虎 with NBODY6++/GPU.