Parallel Computing

Some basic ideas

Amdahl's Law (Gene Amdahl 1967)



Evolution according to Amdahl's law of the theoretical speedup of the execution of a program in function of the number of processors executing it, for different values of p. The speedup is limited by the serial part of the program. For example, if 95% of the program can be parallelized, the theoretical maximum speedup using parallel computing would be 20 times.

By Daniels220 at English Wikipedia - Own work based on: File:AmdahlsLaw.png, CC BY-SA 3.0, https://commons.wikimedia.org/w/index.php?curid=6678551

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 T_{seq} is normalized to unity (1), and can be expressed as:

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

The parallel computing time Tpar under ideal conditions (ideal load balancing, ultrafast communication):

 $T_{par} = X/p + (1-X)$ with processor number (core number) p; Then the speed-up of the program S = T_{seq} / T_{par}:

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

Note: $T_{par}/T_{seq} = 1/S$ (sometimes also plotted) Note the limit of S for p>>1 and X~1 is very large: S = 1/(1-X). $S \sim p$ With communication overhead:

 $T_{par} = X/p + (1-X) + T_{comm} \rightarrow S = 1 / (1-X+X/p+T_{comm})$

If T_{comm} independent of p we have for large p: $S = 1 / (1 - X + T_{comm}) = const.$ If $T_{comm} = c p^k$ (k>0) we get: $S = 1 / (1 - X + c p^k) \rightarrow 0$ for large p!!!

Parallel code on cluster



Strong and Soft Scaling

Strong Scaling: Fixed Problem size, increase p
 Soft Scaling: Increase Problem size, increase p
 (constant amount of work per processing element)

Ansatz for Soft Scaling (T_comm_neglected here): \Rightarrow T_{seq} = p (X + (1-X)) \Rightarrow T_{par} = X + p (1-X) If X~1: p>>1 : \rightarrow T_{seq} ~ pX ; T_{par} ~ X \Rightarrow S = T_{seq}/T_{par} ~ p

ΦGPU – NBODY Code

Speed [Tfloys]



National Astronomical Observatories, CAS

350 Teraflop/s 1600 GPUs . 440 cores = 704.000 GPU-Cores Using Mole-8.5 of

or IPE/CAS Beijing

<u>Berczik et al.</u> 2013







 Table 1
 Main components of NBODY6++

Description	Timing	Expected scaling		
	variable	N	N_p	Fitting value [sec]
Regular force computation	$T_{\rm reg}$	$\mathcal{O}(N_{\mathrm{reg}}\cdot N)$	$\mathcal{O}(N_p^{-1})$	$(2.2 \cdot 10^{-9} \cdot N^{2.11} + 10.43) \cdot N_p^{-1}$
Irregular force computation	$T_{ m irr}$	$\mathcal{O}(N_{\mathrm{irr}} \cdot \langle N_{nb} \rangle)$	$\mathcal{O}(N_p^{-1})$	$(3.9 \cdot 10^{-7} \cdot N^{1.76} - 16.47) \cdot N_p^{-1}$
Prediction	$T_{\rm pre}$	$\mathcal{O}(N^{kn_p})$	$\mathcal{O}(N_p^{-kp_p})$	$(1.2 \cdot 10^{-6} \cdot N^{1.51} - 3.58) \cdot N_p^{-0.5}$
Data moving	$T_{\rm mov}$	$\mathcal{O}(N^{kn_{m1}})$	$\mathcal{O}(1)$	$2.5 \cdot 10^{-6} \cdot N^{1.29} - 0.28$
MPI communication (regular)	$T_{ m mcr}$	$\mathcal{O}(N^{kn_{cr}})$	$\mathcal{O}(kp_{cr} \cdot \frac{N_p - 1}{N_p})$	$(3.3 \cdot 10^{-6} \cdot N^{1.18} + 0.12)(1.5 \cdot \frac{N_p - 1}{N_p})$
MPI communication (irregular)	$T_{ m mci}$	$\mathcal{O}(N^{kn_{ci}})$	$\mathcal{O}(kp_{ci} \cdot \frac{N_p - 1}{N_p})$	$(3.6 \cdot 10^{-7} \cdot N^{1.40} + 0.56)(1.5 \cdot \frac{N_p - 1}{N_p})$
Synchronization	$T_{ m syn}$	$\mathcal{O}(N^{kn_s})$	$\mathcal{O}(N_p^{kp_s})$	$(4.1 \cdot 10^{-8} \cdot N^{1.34} + 0.07) \cdot N_p$
🔶 Sequential parts on host	$T_{\rm host}$	$\mathcal{O}(N^{kn_h})$	$\mathcal{O}(1)$	$4.4 \cdot 10^{-7} \cdot N^{1.49} + 1.23$



Huang, Berczik, Spurzem, Res. Astron. Astroph. 2016, 16, 11. Fig. 2 The speed-up (S) of NBODY6++ as a function of particle number (N) and processor number (N_p). Solid points are the measured speed-up ratio between sequential and parallel wallclock time, dash lines predict the performance of larger scale simulations further. The symbols used in figure have the magnitudes: $1k = 1,024, 1M = 1k^2$ and $1G = 1k^3$.

Roofline Performance Model (LBL)

https://crd.lbl.gov/divisions/amcr/computer-science-amcr/par/research/roofline/

Arithmetic Intensity

The core parameter behind the Roofline model is Arithmetic Intensity. Arithmetic Intensity is the ratio of total floating-point operations to total data movement (bytes).



Research Group at George Washington University: <u>https://lorenabarba.com/</u>

http://lorenabarba.com/wp-content/uploads/2012/01/roofline_slide.png

