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How to build and use special purpose PC clusters in stellar dynamics

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1. The challenge

Large scale, direct particle-particle, brute force N-body simulations are required to accurately resolve numerically transport processes of energy and angular momentum due to two-body relaxation, and interactions between supermassive black holes and other particles having a much smaller mass. Direct accurate N-body codes are the widely used tool for such simulations, e.g., NBODY4 or NBODY6 (Aarseth 1999, 2003), see also Harfst *et al.* (2007) for a less complex code variant, used for benchmarks in this paper. Makino (2002) has presented another direct N-body summation code, which is optimized for a quadratic layout of processor (p required to be a square number).

2. The cluster hardware at RIT and ARI

Computing clusters incorporating the micro-GRAPE-6A boards (see Makino, this volume, for GRAPE) have been installed at the Rochester Institute of Technology (RIT, 'gravitySimulator') and the Astronomisches Rechen-institut (ARI) at the University of Heidelberg (project GRACE = GRAPE + MPRACE). Both clusters consist of 32 compute nodes plus one head node. In addition to a standard Gbit-ethernet, the nodes are connected via a low-latency Infiniband network with a transfer rate of 10 Gbit/s (ARI: 20 Gbit/s). The total, theoretical peak performance is approximately 4 Tflop/s, given by the combined speed of the 32 micro-GRAPE-6A boards. In addition to that the ARI cluster is equipped with reconfigurable FPGA cards (called MPRACE) in addition to GRAPE. MPRACE is optimized to compute neighbour forces and other types of forces between particles such as used for SPH or e.g. molecular dynamics.

It is a relatively new approach to address the challenges of high performance computing by the use of reconfigurable logic, i.e., architectures based on FPGAs (Field Programmable Gate Array). FPGAs mainly consist of a matrix of programmable logic elements plus an interconnecting routing network. Both of them can be configured in a fraction of a second by software, which is minimal compared to typical computing times. We think that the use of reconfigurable logic, presently a relatively new approach to high-performance computing and its power should increase dramatically in the future (Hamada *et al.* 2005; Nakasato *et al.* 2007).

3. Discussion, summary and outlook

Here we show the result of benchmark simulations for a Plummer model on the two clusters. Different models and detailed discussion can be found in Harfst *et al.* (2007). We have varied processor number and particle number. It is a robust result that at one million particles and 32 nodes used, our clusters achieve a sustained performance of 50 %

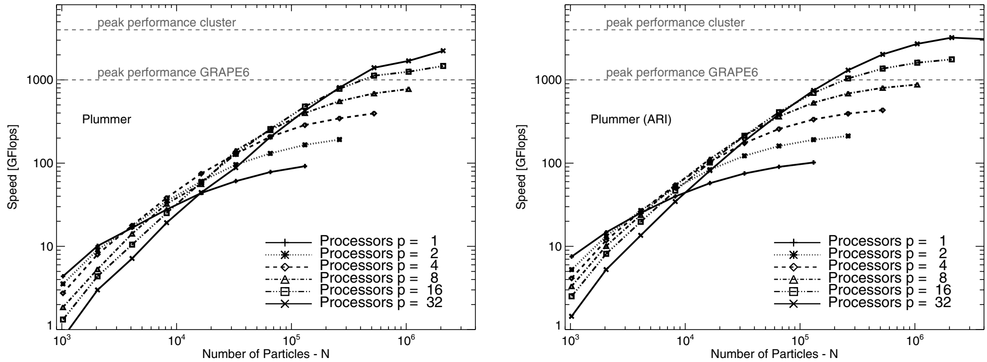

Figure 1. Speed *vs.* particle numbers N for different numbers of processors p. The plots show the results for a Plummer model on the RIT (*left*) and the ARI cluster (*right*).

to 100 % of the peak performance. The total computing time required, and the achieved fraction of the peak performance depend on the details of the astrophysical model, e.g., whether the system is more or less cuspy in central density. The latter will influence the time step structure, and this in turn will affect the parallel run performance. As our complex and communication intensive code typically reaches only a few per cent of peak performance in general purpose parallel computers (e.g., IBM Jump at FZ Jülich), it means that our clusters at RIT and ARI compete in delivered, sustained performance for our application with the top of the list of fastest computers in the world (presently at 280 Tflop/s) at a small fraction of the cost.

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