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Application of a parallel computer system to polymer calculations*

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The LCAP (loosely coupled array of processors) parallel processing systems developed at IBM Kingston have been employed in the simulation of Brownian dynamics on ring polymers. Significant speedups over the serial version of the FORTRAN code have been obtained by using bulk shared memories to expedite information passing between the attached array processors. In this manner we have been able to obtain data for chains with 128 and 256 units. Data on these larger chains indicate that the radius of gyration follows the predicted power law.

Key words: Polymer-Brownian dynamics — Scaling — Parallel processing

Introduction

It is now commonplace to examine polymer properties in terms of scaling ideas [1]. In a recent article Bishop and Michels [2] studied bead size effects on the excluded volume of model linear and ring polymers by Brownian dynamics. Kremer et al. [3] and Webman et al [4] had predicted that the mean square radius of gyration, $\langle S^2 \rangle$, of chains follows a scaling relation with scaling variable $X = N(\sigma/l)^{d/\phi}$, where N is the number of beads (units) on the chain, σ is the

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bead size, l is the link length, d is the dimension and ϕ is the crossover exponent from Gaussian to nontrivial behavior. The scaling law in $\langle S^2\rangle/\langle S_0^2\rangle \sim X^{2\nu-1}$ for $X \to \infty$ where ν, is the critical exponent for the mean dimensions of an isolated polymer chain, $\langle S_0^2\rangle$.

Assuming the values appropriate for three-dimensions, $\nu \cong 0.60$ and $\phi = 0.50$, the scaling relations become

$$X = N(\sigma/l)^6; \langle S^2\rangle/\langle S_0^2\rangle = AX^{0.20} \tag{1}$$

Bishop and Michels [2] found excellent agreement between their data on linear chains and the scaling prediction for a variety of N and (σ/l) values. However, the data on rings showed some deviation from the predicted exponent. They commented that this difference could mean that rings take longer to reach their asymptotic limit because of the ring constraint.

In this note we examine the scaling relations for larger ring polymers by using the IBM Kingston LCAP facility, developed by Enrico Clementi, to generate the configurations.

Method

Ring polymers have been simulated by the Brownian dynamics method of Michels and Wiegel [5]. N beads are joined together by nearest neighbor harmonic spring forces. Each bead is subject to a random force and a frictional force proportional to the velocity. Excluded volume chains also have a Lennard-Jones force acting between all particles. The range of this force has been set to $2^{1/6}\sigma$ so as to include only the repulsive part of the potential. The polymer is started in a square configuration and its equations of motion are solved using Verlet's [6] method. The configuration data were split into six batches and batched means and standard deviations were calculated. Runs have been made for $N = 128$ and 256 with $\sigma = 1.0$, 0.75 and 0.0. Data have been obtained for $\langle S^2\rangle$. All results are contained in Table 1.

The data obtained in this study were generated on the IBM Kingston LCAP system. The generic structure of this system incorporates an IBM host mainframe (either an IBM 3081 or 3084) coupled by IBM 3 Mbtye/s channels to up to ten FPS-X64 attached array processors. This master-slave configuration is augmented by providing tight coupling between the FPS processors through the inclusion

Table 1. The simulation results

N	σ	$\langle S^2\rangle$
128	0.00	11.11 ± 0.60
	0.75	32.05 ± 0.82
	1.00	41.17 ± 1.58
256	0.00	24.07 ± 1.46
	0.75	77.36 ± 1.85
	1.00	104.36 ± 2.25

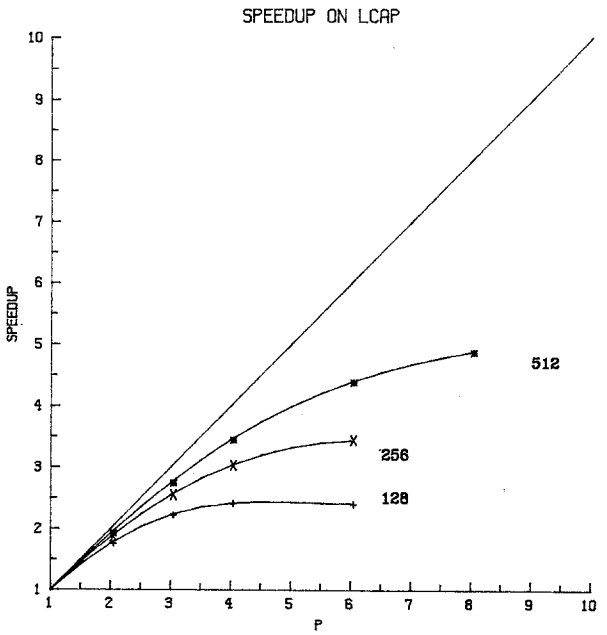

Fig. 1. Speedup on the LCAP system. P is the number of processors

of six shared memories. Five of these are 32 Mybtes in size. These units are multiplexed four ways so as to structure the ten processors in a doubly connected ring configuration. The sixth unit is a global 512 Mbyte memory that is multiplexed twelve ways in order to directly couple all ten processors. The peak bandwidth of the smaller memories is 44 Mbyte/s and that of the larger is 132 Mbyte/s. In addition, all the processors are coupled by a fast bus (22 Mbtye/s) which provides useful message passing and broadcast capabilities.

Brownian dynamics simulations such as those reported here are very computationally intensive because larger chains take longer to equilibrate from their initial configuration. Moreover, the configurations need to be saved at a larger time spacing in order to diminish the correlation in the data. Typically, we discarded 90 000 steps for equilibration and saved data every 5000 steps.

In order to be able to employ the LCAP parallel computer system we first needed to change the serial FORTRAN code. This code has a variety of modules: a main driver to call the other routines, an initial setup routine, a random force routine, a harmonic force routine, a Lennard-Jones force routine, a Verlet integration routine and a sample routine to dump configurations. Since the evaluation of the force on bead i is independent of the evaluation of the force on bead j, all the force routines can be made parallel [7]. Moreover, the integration routine can also be made parallel.

The division of labor among processors was such that each was responsible for calculating the harmonic and random forces on an unique portion of the ring polymer. For the Lennard-Jones force each processor executed a segmented

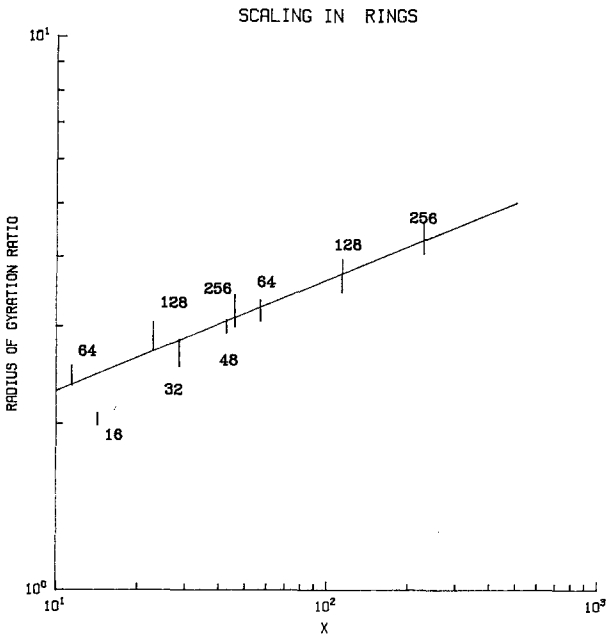

Fig. 2. Scaling for rings

fraction of the double Do loop over all two body terms. Synchronization at the end of each time step was accomplished by having each processor write to shared memory its contribution to the displacements of the original coordinates. These results were then summed to give the new coordinates for the beginning of the next time step.

After changing the code we performed speedup tests. The speedup, S, equals T_1/T_p, where T_p is the time required to perform a calculation with p processors and T_1 is the time needed on a uniprocessor. Figure 1 presents the results for $N = 128$, 256 and 512. It is clear that large problems can effectively utilize the power of the LCAP system.

Results

The ratios $\langle S^2\rangle/\langle S_0^2\rangle$ have been computed from the data in Table 1 and are presented in Fig. 2. The error bars of the ratios have been determined from the error bars in the numerator and denominator by the usual formula for statistically independent errors. Bead size/bond length ratios of 0.98 and 0.75 were used. Also plotted in Fig. 2 are the data of Bishop and Michels [2] for $N = 16$, 32, 48 and 64. The straight line has been drawn with slope 0.20. Figure 2 indicates that high values of X ($X > 20$) are consistent with the scaling prediction of an exponent of 0.20.

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