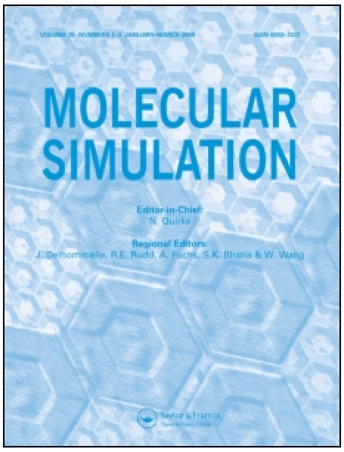

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Long Memory Effects in the Stress Correlation Function

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LONG MEMORY EFFECTS IN THE STRESS CORRELATION FUNCTION

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The stress correlation function (SCF) in a one-dimensional cellular automata-fluid is calculated by computer simulations upto 3000 time steps. The results are compared with the 1-D tails $t^{-1/2}$ and $t^{-2/3}$ of bare (BMC) and self-consistent (SCMC) mode coupling theories. The crossover between both tails is estimated to occur after $t_{\rm cross} \simeq 35000$ time steps. For $t < 400$ and systems with $L \geq 500$ sites there is good agreement with BMC-theory for finite systems. For $t > 400$ there are signs of faster-than-$1/\sqrt{t}$-decay in the SCF. The simulated data for the "divergent" transport coefficient at times $t > 400$ are analyzed in terms of a crossover function, constructed from SCMC-theory. However a quantitative verification of the SCMC-theory is still out of reach.

KEY WORDS: Stress correlation function, long time tail, mode coupling theory

1 INTRODUCTION

Cellular Automata (CA) fluids [1] have advantages as well as disadvantages over ordinary continuous models for simulating large systems over long intervals of time. The advantages stem in part from the discrete nature of time, velocity and position variables and in part from a time evolution that can be treated advantageously with parallel processor algorithms. The main disadvantages are the occurrence of large fluctuations in any given initial configuration, thus requiring that averages be taken over large numbers of such configurations. For the velocity correlation function this can be achieved by a very ingenious algorithm, called moment propagation method [2, 3]. For other correlation functions efficient algorithms are still lacking.

The equilibrium time correlation functions are important quantities that require simulations on large scale systems over long intervals of time. The velocity autocorrelation function (VACF) describes single particle dynamics; the stress-stress correlation function (SCF) collective dynamics. Both functions are of fundamental importance for the understanding of relaxation phenomena in fluids, in particular of long memory effects. A lot of effort has been put into simulating the SCF for continuous fluids with the aim of studying its long time effects and to test the standard [4] and extended mode coupling theories [5]. The basic difficulty is well described by Ladd *et al.* [6], and we quote: "... statistical errors and finite size effects, associated with interference between sound waves make it very expensive computationally to obtain sufficiently accurate data for a stringent test of the theory."

According to the standard unrenormalized or bare mode coupling (BMC) theory, the correlation functions $\varphi(t)$ in d-dimensional systems have long time tails decaying as $At^{-d/2}$. However, in 1- and 2-dimensions this algebraic decay gives rise to divergent transport coefficients and the theory is therefore inconsistent, at least for superlong times. An estimate for the superlong time behavior can be obtained by introducing time dependent transport coefficients, imposing that the mode coupling theory be self consistent, and determining the asymptotic solution of the self consistent theory. The resulting superlong time tails are:

$$\varphi(t) \sim \begin{cases} (t\sqrt{\ln t})^{-1} & \text{(2 dimensions)} \\ t^{-2/3} & \text{(1-dimension).} \end{cases} \tag{1}$$

To what extent have these theoretical predictions been confirmed by computer simulations? The VACF in CA-fluids from 1 up to 4 dimensions has been simulated with very high statistical accuracy using the moment propagation method, and the predictions of bare mode coupling theory have been confirmed in great detail for intermediate time ranges, even in one dimension where the VACF does not have an algebraic tail, but decays exponentially [7].

To observe the superlong time tails the divergent contributions to a transport coefficient should exceed its Boltzmann (bare, unrenormalized, short-time) value. From this observation van der Hoef and Frenkel [8, 9] estimate that in two-dimensional CA-fluids the crossover from the bare $1/t$-tail to the superlong tails in (1) occurs after 10^{18} time steps. Therefore it is not possible to detect this crossover with present day computational power. However the authors did observe a renormalization of the tails, showing faster-than-$1/t$-decay. This behavior could be estimated reasonably well using mode coupling theory with time dependent transport coefficients.

Computer simulations on the SCF axe essentially lacking, apart from some inconclusive short time simulations for a one-dimensional CA-fluid [10]. Therefore none of the above mode coupling predictions, not even the exponent $d/2$ of the bare mode coupling theory, have ever been tested and compared with computer simulations on CA-fluids. The reason is that the moment propagation method with its high statistical accuracy is not applicable to the SCF. Consequently only standard molecular dynamics techniques are available to measure this function. As lattice gas simulations are very noisy, simulations of reasonable statistical accuracy are not feasible in 2- and 3-dimensional CA-fluids [11, 12]. For continuous fluids the situation is essentially the same [13]. We remind the reader that computer simulations of the long time behavior of the SCF, in particular of its collisional transfer parts, seem to be in conflict with the predictions of standard mode coupling theory. A second possibility is that computer simulations have not yet reached the asymptotic time regime.

What about one dimension? To obtain an estimate for the crossover time from a bare $t^{-1/2}$-tail to the superlong $t^{-2/3}$-tail we use the same arguments as in Ref. [8, 9]. The crossover time is found to be 3.5×10^4 and 10^5 time steps at relative densities of 10% and 20% respectively. The tentative conclusion is that it might be feasible to accurately measure the bare $t^{-1/2}$-tails, and possibly even faster-than-$t^{-1/2}$-decay provided the systems are large enough to eliminate finite size effects, such as interference effects from the sound waves in the periodic replicas of the system [7]. This paper gives a preliminary account of our findings.

II MODEL AND MODE COUPLING THEORY

We consider the CA-fluid, introduced by d'Humieres *et al.* [14] and studied extensively in Ref. [7]. The system under consideration has L lattice points on a line and periodic boundary conditions are imposed. At each site there exist five velocity channels, $c = (-2, -1, 0, 1, 2)$. Each channel can be occupied by at most one particle (Fermi exclusion rule). The collision rules for these particles are self-dual, i.e. invariant under the interchange of particles and holes,

$$\begin{aligned}
(-1) + (1) + (0)^{\dagger} &\Leftrightarrow (-2) + (2) + (0)^{\dagger} \\
(0) + (-1) + (2)^{\dagger} &\Leftrightarrow (-2) + (1) + (2)^{\dagger} \\
(0) + (1) + (-2)^{\dagger} &\Leftrightarrow (-1) + (2) + (-2)^{\dagger}.
\end{aligned} \tag{2}$$

Here $(i)^{\dagger}$ indicates collisions allowed to take place irrespective of the presence of a "spectator" particle with velocity $(i)^{\dagger}$ at the same lattice point. The CA-fluid has two collisional invariants, the number of particles and the total momentum. As a consequence the density $\rho(r,t)$ and flow field $u(r,t)$ are slowly varying in time and the model behaves as a one-dimensional fluid. The long wave length excitations (only sound waves) are approximately described by the linearized hydrodynamic equations with a time dependent longitudinal viscosity or sound damping constant $\nu(t)$, that diverges as t approaches infinity [14],

$$\begin{aligned}
\partial_t \rho(r,t) + \rho \nabla u(r,t) &= 0 \\
\partial_t u(r,t) + (c_0^2/\rho)\nabla\rho &= \nu(t)\nabla^2 u(r,t).
\end{aligned} \tag{3}$$

Here $c_0 = \sqrt{2}$ is the speed of sound. The transport coefficient is given by the Green-Kubo formula [15],

$$\nu(t) = \sum_{\tau=0}^{t}{}^{*} \frac{\langle J(\tau)J(0)\rangle}{\langle P^2\rangle} \equiv \frac{\langle J^2\rangle}{\langle P^2\rangle} \sum_{\tau=0}^{t}{}^{*} \varphi(\tau). \tag{4}$$

Here $\langle \cdots \rangle$ is an average over an equilibrium ensemble, $\varphi(t)$ is the stress-stress correlation function (SCF), normalized as $\varphi(0) = 1$, and the asterisk on the summation sign indicates that the term $\tau = 0$ has a weight 1/2. Furthermore P is the total momentum and J the subtracted momentum flux or stress tensor, defined as

$$P = \sum_{r,c} c\,n(r,c,t)$$

$$J(t) = \sum_{r,c} (c^2 - c_0^2)\,[n(r,c,t) - f], \tag{5}$$

and expressed in terms of the occupation number $n(r,c,t)$ of velocity channel c at site r at time t. Its average value is $\langle n(r,c,t)\rangle = f = \rho/5$, and the averages are $\langle J^2\rangle = 14f(1-f)L$ and $\langle P^2\rangle = 10f(1-f)L$.

The object of main interest is the SCF $\varphi(t)$ and its time sum $\nu(t)$. For short times the SCF decays exponentially through uncorrelated collisions, and its contributions to (4) defined the Boltzmann or bare viscosity [14],

$$\nu_0 = \frac{3}{10f(1-f)} - \frac{7}{10}. \tag{6}$$

For longer times the SCF decays more slowly, as explained by mode coupling theory [17, 16]. Here we quote the different results for the dominant long time behavior, obtained from bare (BMC) and self consistent (SCMC) mode coupling theories. The index (LB) refers to the finite size L and to the BMC-theory:

$$\begin{aligned}\varphi_{\mathrm{LB}}(t) &\simeq \frac{A}{L}\sum_{q\neq 0}\,[1+\cos(2qc_0t)]\exp(-\nu_0q^2t)\\ &\simeq -\frac{2A}{L} + \frac{A}{\sqrt{4\pi\nu_0 t}}\left[1+\sum_{n=-\infty}^{n=\infty}\exp\left[-\frac{c_0^2}{\nu_0 t}\left(t-\frac{1}{2}nt_a\right)^2\right]\right].\end{aligned} \tag{7}$$

Here $t_a = L/c_0$ is the accoustic traversal time and the amplitude A is given by

$$A = 7(1-2f)^2/[200f(1-f)]. \tag{8}$$

The above formula accounts for finite size effects, induced through the discreteness of the reciprocal lattice vector $q = 2\pi m/L\,(m = 0, \pm 2, \ldots \pm L/2)$, where periodic boundary conditions have been imposed. For long times and fixed volume L the first line in (7) can be transformed into the second one [7, 16]. The maxima at $t = \frac{1}{2}nt_a$ are caused by the interference of sound waves coming from periodic replicas of the system. In the thermodynamic limit $(L\to\infty)$ the BMC-result (7) reduces to,

$$\varphi_{\mathrm{B}}(t) = \frac{A}{\sqrt{4\pi\nu_0 t}}\,[1+\exp(-c_0^2t/\nu_0)]. \tag{9}$$

where the second term is negligible for all densities and times of interest $(t > 6)$.

As mentioned in the introduction, the $t^{-1/2}$-tail in the SCF leads according to (4) to a transport coefficient increasing like $\nu(t) \sim \sqrt{t}$. To account for a time dependent transport coefficient within the mode coupling theory, one has to investigate the hydrodynamic equation (3). This yields Eq. (7) with $\nu_0 t$ replaced by $t\bar{\nu} \equiv \int_0^t d\tau\nu(\tau)d \equiv M(t)$, as explained in Ref. [17]. The result is

$$1.4\varphi_{\mathrm{SC}}(t) = M'' = bM^{-1/2}, \tag{10}$$

with $b = 1.4A/\sqrt{4\pi}$. Equation (10) is a self-consistent equation for $M(t)$. The super-long time tail can be determined by substituting $M(t) = at^{\alpha}$ in (10.). This yields for the constant $\alpha = 4/3$ and $a = (9b/4)^{2/3}$. The super-long time tail is then

$$\varphi_{\mathrm{ASC}}(t) \simeq (2b/3t)^{2/3}. \tag{11}$$

III RESULTS

We first consider the finite size effects and compare in particular the second line of (7) with its thermodynamic limit in (9). There are two distinct effects. The first one is the additve constant, $-2A/L$, which comes from excluding the term $q = 0$ from the summation over the reciprocal lattice. In order to be able to observe the $t^{-1/2}$-tail in a finite system, we need to plot the corrected SCF $\hat{\varphi}(t) \equiv \varphi(t) + 2A/L$, both for the simulation data and for the theoretical results in (7). This will be done in all plots in this paper. It is a sizeable correction for small systems, as can be verified for the system with $L = 100$ sites in Figure 1.

The second set of finite size effects are the terms in (7) with $n \neq 0$ in the summation over n, that are caused by the interference of sound waves due to the periodic boundary conditions. At times $t_n = \frac{1}{2}nt_a$, which are half integer multiples of the acoustic traversal time, the finite system result (7) predicts peaks in SCF with a maximum $\hat{\varphi}_{\text{LB}}(t_n) = 2A/\sqrt{4\pi\nu_0 t_n}$, that are independent of L and twice as large as the result for the thermodymic limit. The width of a peak is $\sqrt{\nu_0 t_n}/c_0$. Therefore,

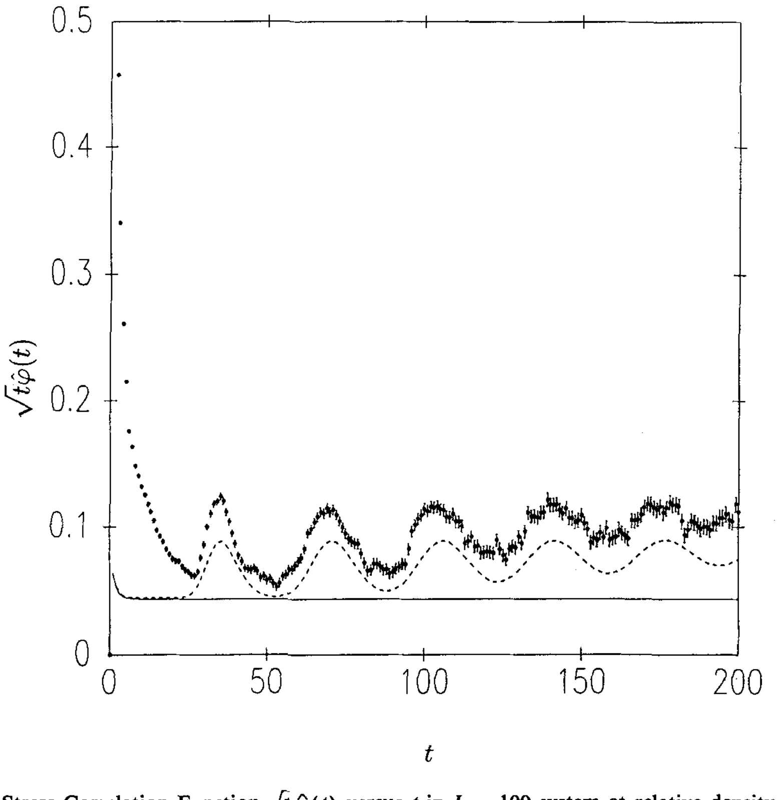

Figure 1 Stress Correlation Function $\sqrt{t}\,\hat{\varphi}(t)$ versus t in $L = 100$ system at relative density $f = 0.1$, averaged over 5×10^6 samples. The simulation results (vertical error bars) are compared with the BMC-results $\sqrt{t}\,\hat{\varphi}_{\text{LB}}(t)$ (dashed line) for a finite system and $\sqrt{t}\,\varphi_{\text{B}}(t)$ (solid line) for an *infinite* system. Here $\hat{\varphi} \equiv \varphi + 2A/L$ denotes the corrected SCF. Peaks occur at multiples of half the accoustic traversal time $\frac{1}{2}t_a = 35.1$.

the observation of the $t^{-1/2}$-tail in finite systems requires that the observation time t be smaller than half the acoustic traversal time. Inspection of the simulation data in Figures 1 and 2 confirms that the peaks are indeed at the predicted locations.

The most important observations are, however, that (i) the simulation results for the $L = 500$ system are in quantitative agreement not only with the asymptotic result for an infinite system $A/\sqrt{4\pi\nu_0 t}$ (solid line) over the time interval $50 < t < 150$, but also with the finite size corrections due to interference of sound waves (dashed line) for $t > 150$, and (ii) that the system of $L = 100$ sites with $5fL = 50$ particles, with its first peak at $\frac{1}{2}t_a = 35.4$, is much too small to observe the $t^{-1/2}$-tail. Furthermore Figure 1 shows that (7) describes the finite size effects only qualitatively. The simulated values at the maxima are about 40% higher than predicted by the theory. This seems an indication that there is extra size dependence in the smaller systems that is not correctly accounted for by the hydrodynamic ingredients of the mode coupling theory. The simulation data for system sizes $L = 100$ and $L = 500$ were obtained by averaging over 5×10^6 samples.

A more quantitative test on the validity of the mode coupling theories is shown in Figure 3, where the simulation data for $\nu(t)$ are plotted for $L = 500$ as a func-

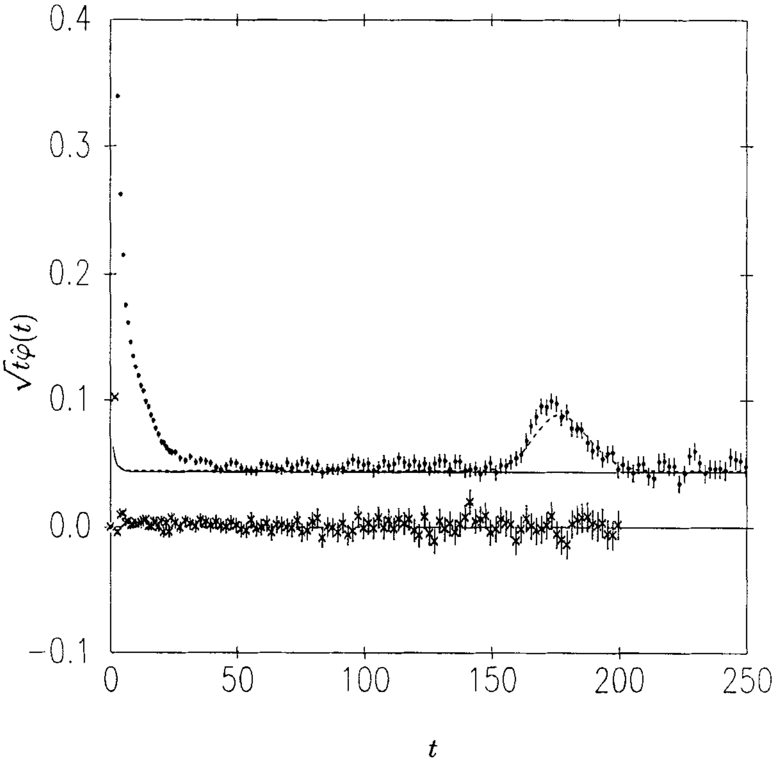

Figure 2 Simulation data for the SCF, $\sqrt{t}\,\hat{\varphi}(t)$, averaged over 1.5×10^6 samples in an $L = 500$ system at densities $f = 0.1$ (dots) and $f = 0.5$ (crosses), show absence of a long time tail for the half filled lattice. The sound wave interference peak occurs at $\frac{1}{2}t_a \simeq 177$. The solid/dashed lines represent BMC-results for infinite/finite systems.

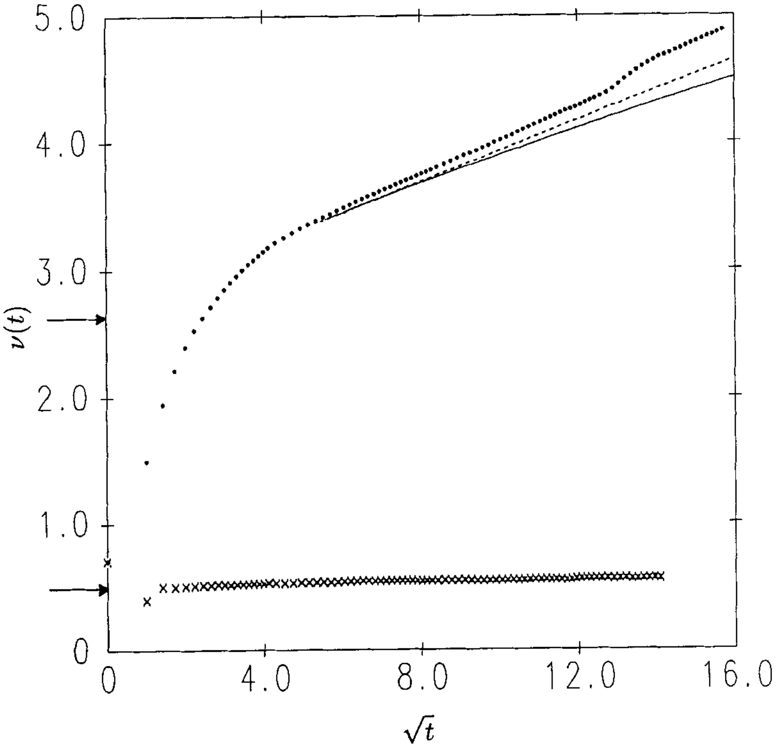

Figure 3 Time dependent viscosity $\nu(t)$ versus $\sqrt{t}$ in $L = 500$ system at densities $f = 0.1$ (dots) and $f = 1/2$ (crosses). The plateau value at $\nu \simeq 1/2$ indicates the absence of a long time tail at $f = 1/2$. As for solid and dashed lines, see the text and Figure 5.

tion of $\sqrt{t}$ at densities $f = 0.5$ and $f = 0.1$. In the half filled lattice ($f = 1/2$) the long time tail in (7) vanishes ($A = 0$) (see also Figure 2 for $f = 0.5$) and $\nu(t)$ reaches a plateau value of $\nu_{\text{SIM}}(\infty) \simeq 0.55$, to be compared with the unrenormalized Boltzmann value $\nu_0 = 0.5$. At short times ($t = 1, 2$) the exact values of SCF $\varphi(t)$ are given by their Boltzmann approximation, $\varphi(1) = -3/14$ and $\varphi(2) = +1/14$. With the help of Equation (4) we obtain the theoretical values $\nu(0) = 0.7$, $\nu(1) = 0.4$ and $\nu(2) = 0.5$, in excellent agreement with the simulation data in Figure 3. For $f = 0.1$ the long time tail has a nonvanishing amplitude and $\nu(t)$ keeps increasing with time. The BMC-theory predicts a straight line. Figure 4 shows the simulation data for the $L = 2000$ system at reduced density $f = 0.1$, obtained by averaging over 3×10^6 and compared with the result (9) for the infinite system (solid line). There is good agreement with BMC-theory for times $50 < t < 400$. For times in the range of 400 to 600 steps we see the first indication of a faster-than-$t^{-1/2}$-decay, as implied by the SCMC-theory. We recall that the first interference peak due to finite size effects occurs at $t \simeq 707$.

To quantify the renormalization of the BMC-tail we show in Figure 5 the time dependent viscosity $\nu(t)$ versus $\sqrt{t}$, as measured in the simulations on the $L = 2000$

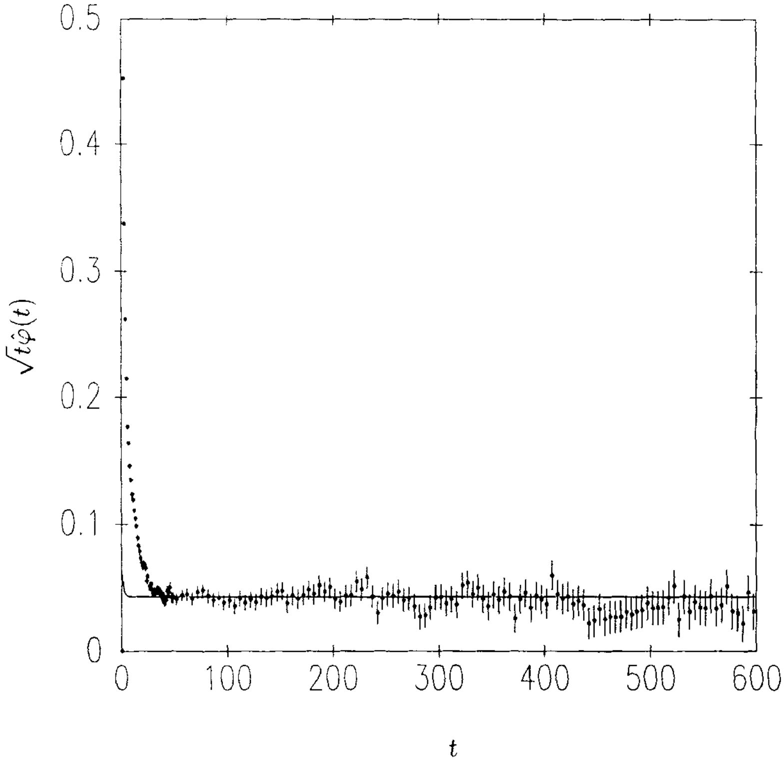

Figure 4 Stress Correlation Function $\sqrt{t}\,\varphi(t)$ at $L = 2000$ ($\frac{1}{2}t_a = 707$) and $f = 0.1$, averaged over 3×10^6 samples. Simulation results (vertical error bars) are compared with the BMC-results $\varphi_B(t)$ (solid line) for an infinite system. Finite size effects are negligible. For $t > 400$ the data show signs of faster-than-$1/\sqrt{t}$-decay.

system. During the time interval covered by the simulations $\nu(t)$ increases from the Boltzmann value, $\nu_0 = 2.63$, reached around $t = 6$, to about $2\nu_0$ at $t = 600$. Consequently, the tail (10) in the self-consistent theory is about a factor $1/\sqrt{2} = 0.7$ smaller than in the BMC-theory. This theoretical prediction is consistent with the simulation data, as shown in Figure 4 and Figure 5. However, better statistics is required to confirm or disprove the quantitative predictions.

In the simulations on the $L = 2000$ system in Figure 4 renormalization of the BMC-effects start to become noticeable in the time interval of 450 to 600. One therefore needs longer time runs, which implies larger system sizes. We have therefore considered a system of $L = 10000$ sites at reduced density $f = 0.1$ where the interference peak due to sound waves would appear at $\frac{1}{2}t_a = 3540$. Figure 6 and Figure 7 show the results obtained by averaging over 4×10^6 initial configurations. These simulations took 500 hours of CPU time on a Hitac M680. The number of samples is a factor 10 smaller than in the $L = 2000$ system. Unfortunately, the large statistical fluctuations make it impossible to observe a faster-than-$t^{-1/2}$-decay in the $L = 10000$ system.

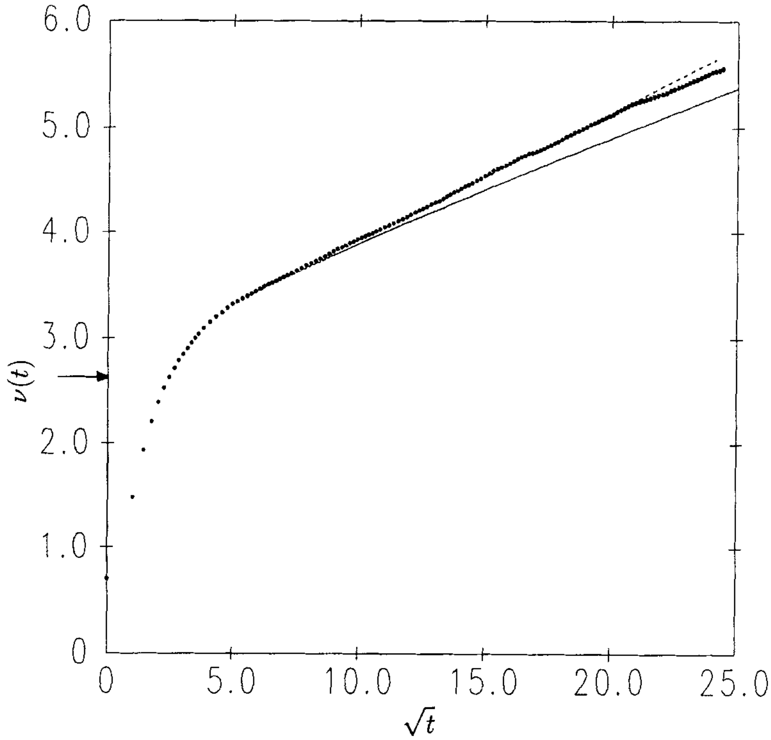

Figure 5 Simulated value of the time dependent viscosity $\nu(t)$ versus $\sqrt{t}$ at $f = 0.1$ for the $L = 2000$ system, compared with the crossover function (solid lines) and the integrated tails of BMC-theory (dashed lines) determined from initial conditions at $t_1 = 30$. The horizontal arrow on the y axis marks the Boltzmann value $\nu_0 = 2.63$, reached at $t \simeq 6$.

Clearly the statistical noise in the sum function $\nu(t)$ in (4) is much smaller than that in SCF $\varphi(t)$ itself. The question arises: are there any possibilities of testing the BMC-and the SCMC-theories using the $\nu(t)$-data? For that purpose we subtract the short time "instantaneous" Boltzmann constribution from ν_0, i.e.

$$\Delta\nu(t) = \nu(t) - \nu_0 \simeq Bt^{\beta}, \tag{12}$$

and analyze this difference in terms of an exponent β. In the calculation of $\nu(t)$ we have used the corrected SCF, $\hat{\varphi} = \varphi + 2A/L$, considered above, in order to eliminate finite size effects that could possibly mask power law behavior. In Figure 8 the quantity $\log(\Delta\nu(t))$ is plotted versus $\log(t)$. The slope β in the $L = 2000$ system is measured over the time interval $(t_1, 600)$ yielding $\beta = 0.46$ ($t_1 = 50$, 100) and 0.42 ($t_1 = 300$). The corresponding values in the $L = 10000$ system are $\beta = 0.47$ ($t_1 = 50, 100, 300, 500$) and 0.48 ($t_1 = 1000$). The exponent is very close to the prediction of the BMC-theory. This is consistent with the very large crossover to the superlong time tail after 35000 time steps.

A more quantitative comparison with the SCMC-theory can be obtained by analyzing the simulation data in terms of the crossover function, $M(t) = \Sigma_{s=0}^{t} \nu(s)$, at finite times. The second order differential equation for $M(t)$ in (10) can

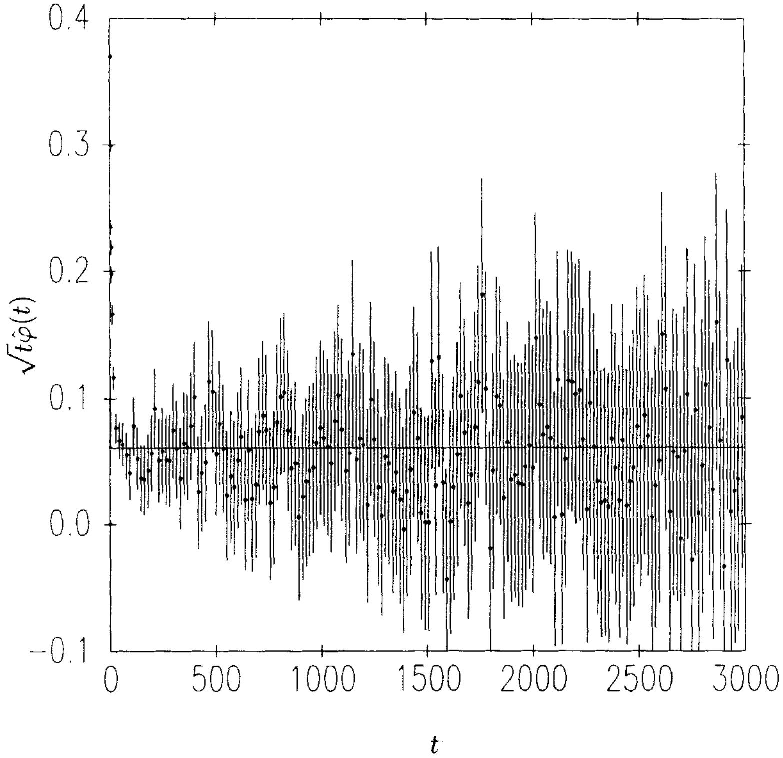

Figure 6 Same comparison as in Figure 4 for $L = 10000$ system ($\frac{1}{2}t_a = 3540$). Simulation data are averaged over 4×10^6 samples.

be solved by quadrature. The integration constants are fixed by taking the values $M(t_1)$ and $M'(t_1) = \nu(t_1)$ from the simulation data at a time t_1, where BMC-theory applies. Inspection of Figure 2 and Figure 4 shows that this is approximately the case for $t_1 = 30$, and we have taken $M(30)$ and $\nu(30)$ from the high accuracy simulation data for the $L = 2000$ system. The agreement of the crossover function $\nu(t)$ (solid line) in Figure 3 ($L = 500$) and Figure 5 ($L = 2000$) with the simulation data of high statistical accuracy is very good for $t < \frac{1}{2}t_a$. The simulation data for $\nu(t)$ in Figure 7 $L = 10000$) have a much lower statistical accuracy. The solid line represents the same crossover function as used in Figure 3 and Figure 5. It increases more slowly than the simulation data. If we fix the integration constants, $M(t_1)$ and $M'(t_1)$, from the simulation data for the $L = 10000$ system at $t_1 = 50$, 100 or 500, the crossover function and simulation data agree slightly better. To suppress statistical fluctuations the slope $M'(t_1)$ has been replaced by the average slope over intervals of 60 around t_1.

For compaprison we have also plotted (dashed lines) in Figures 3, 5 and 7 the integrated tail (9) of the BMC-theory, i.e.

$$\nu(t) - \nu(t_1) \simeq \frac{1.4A}{\sqrt{4\pi\nu_0}}(\sqrt{t} - \sqrt{t_1}), \tag{13}$$

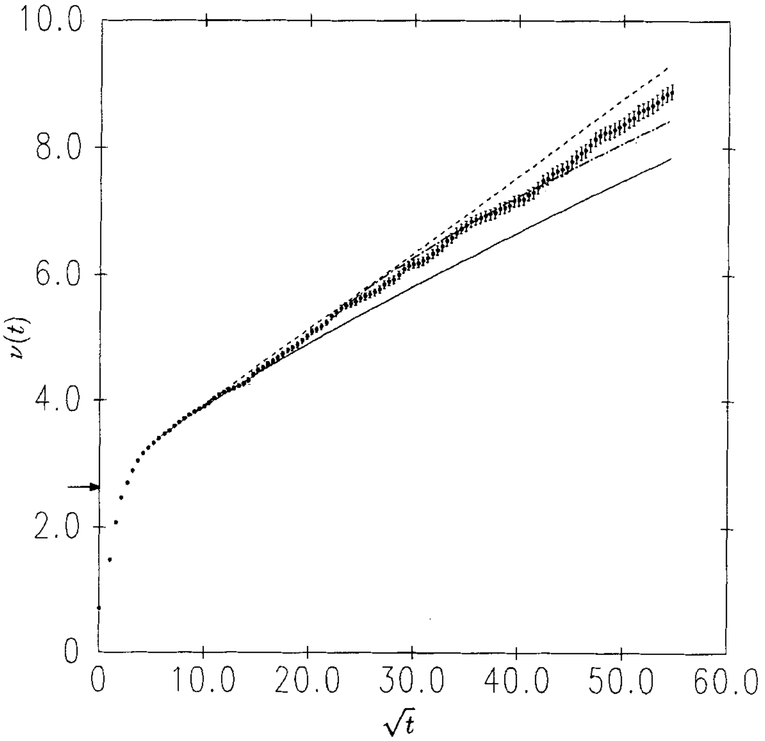

Figure 7 Simulated value of the time dependent viscosity $\nu(t)$ versus $\sqrt{t}$ at $f = 0.1$ for the $L = 10000$ system. The horizontal arrow on the y-axis marks the Boltzmann value $\nu_0 = 2.63$. The solid and dashed lines are the same as those in Figure 5. The dash-dotted line shows the crossover function determined from initial condition at $t_1 = 500$ for $L = 10000$ system.

where $t_1 = 30$ is chosen as the approximate time where BMC-theory sets in Figure 5 gives a confirmation that a slightly slower growth starts to become visible arround $t = 400$, which we already mentioned in the discussion of the SCF in Figure 4. Figure 7 for the large system is consistent with this trend. Figure 3 suggests again that finite size effects in $\nu(t)$ may be quite large in a small system with $L = 500$ sites, that contains only $5fL = 250$ particles. They are not correctly described by the mode coupling theories and not yet understood.

On the basis of our low statistical accuracy it is premature to conclude that either the SCMC-theory only sets in for later times, somewhere between 100 and 500, or that its predictions for very long times are in conflict with the simulation data. In order to draw any more definite conclusions our statistical accuracy for the $L = 10000$ system has to be increased.

IV CONCLUSIONS AND DISCUSSION

1. The stress-stress correlation function (SCF) has been studied in a one-dimensional fluid-type cellular automaton, where sound waves are the only long

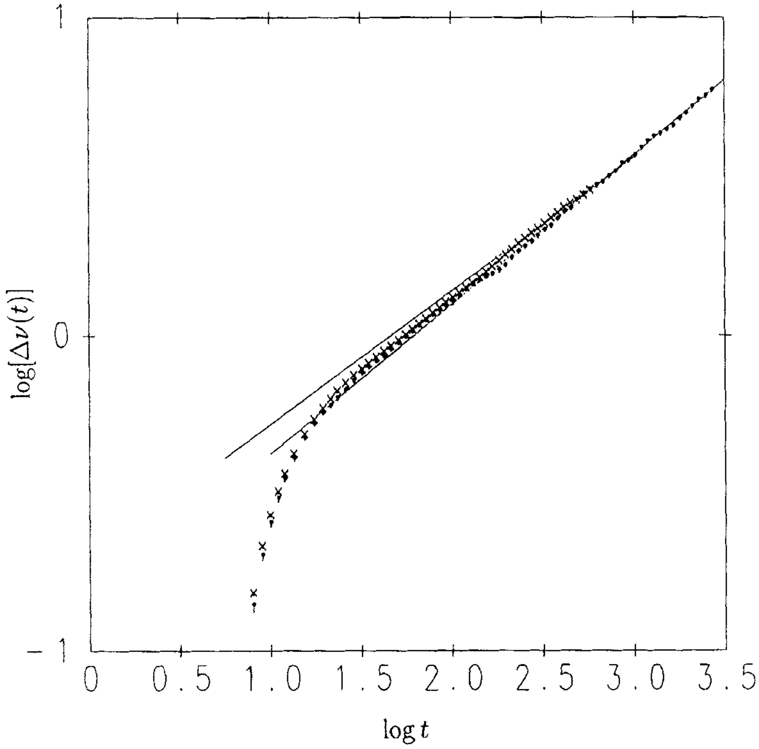

Figure 8 Exponents β, defined as $\Delta\nu(t) \sim t^{\beta}$, determined from the simulation data for $L = 2000$ and $L = 10000$. Straight lines show the slopes $\beta = 0.42$ ($L = 2000$, $t_1 = 300$) and 0.47 ($L = 10000$), respectively.

wave length excitations, using mode coupling theories and computer simulations. The simulations were carried out by the Hitac M680 system at the Center of Information Science of Senshu University.

2. For the first time the simulations of the SCF have sufficient statistical accuracy to measure a $t^{-1/2}$-tail in the time interval $50 < t < 400$, 400, in quantitative agreement with the bare mode coupling (BMC) theory, where transport coefficients are given by their Boltzmann values.

3. There are strong finite size effects in systems with $L = 100$ and $L = 500$ sites, containing respectively 50 and 250 particles. There are very pronounced interference peaks at half integer multiples of the accoustic traversal time, L/c_0, as visible in Figures 1 and 2. If L is not too small the BMC-theory describes the finite size effects correctly. The results can thus be used to design appropriate computer experiments.

4. In the time interval $400 < t < 600$ in a system of $L = 2000$ sites we have observed faster-than-$t^{-1/2}$-decay, that is consistent with the predictions of self consistent mode coupling (SCMC) theory. Our statistical accuracy, obtained by averaging over 3×10^6 runs, is however still too poor to make quantitative comparisons. For larger systems ($L = 10000$) we lack sufficient accuracy to draw any conclusions.

5. The asymptotic behavior of the SCMC-theory (the so-called superlong time tail) has the form SCF $\varphi(t) \sim t^{-2/3}$. The crossover to this tail is estimated to occur after 3×10^4 or 10^5 time steps at relative densities of respectively 10% or 20%. This seems to be outside the time range accessible by present day computer simulations.

6. SCMC-theory allows us to construct explicitly a crossover function for $\nu(t)$ between the $t^{1/2}$-tail of BMC-theory and the superlong $t^{1/3}$-tail of SCMC theory. The crossover function for $\nu(t)$, constructed from the simulation data after $t_1 = 30$ time steps, agrees rather poorly with the simulation data at very large times. If $t_1 = 30$ is increased to $t_1 = 500$ the agreement is good over the whole time interval upto 3000 time steps. This demonstrate that large integration constants in sum functions, that can not be estimated theoretically, make $\nu(t)$ rather unsuitable to test SCMC-theory.

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