

## **Dynamic Critical Exponent of the BFACF Algorithm for Self-Avoiding Walks**

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We study the dynamic critical behavior of the BFACF algorithm for generating self-avoiding walks with variable length and fixed endpoints. We argue theoretically, and confirm by Monte Carlo simulations in dimensions 2, 3, and 4, that the autocorrelation time scales as  $\tau_{\text{int},N} \sim \xi^4 \sim \langle N \rangle^{4\nu}$ .

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**KEY WORDS:** Self-avoiding walk; polymer; Monte Carlo; BFACF algorithm; dynamic critical exponent.

In recent years there has been a widespread use of dynamic Monte Carlo methods as a tool for studying the static properties of statistical-mechanical systems.<sup>(1,2)</sup> These studies have, however, been hampered by critical slowing-down:<sup>(3)</sup> the autocorrelation time  $\tau$  of the Monte Carlo stochastic process grows to infinity as the critical point is approached, which leads to a corresponding growth in the statistical error bars.

In this paper we study the dynamic critical behavior of an algorithm for simulating self-avoiding walks (SAW) with variable length and fixed endpoints, due to Berg and Foerster<sup>(4)</sup> and Aragão de Carvalho, Caracciolo, and Fröhlich,<sup>(5,6)</sup> hereafter called BFACF. For the SAW, criticality corresponds to the long-chain limit. The autocorrelation time of the Monte Carlo stochastic dynamics behaves asymptotically as

$$\tau \sim \langle N \rangle^p \tag{1}$$

where  $N$  is the number of steps in the walk. This defines a dynamic critical exponent  $p$  which is the object of this study.

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This paper is dedicated to our friend and colleague Jerry Percus on the occasion of his 65th birthday.

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Let us give a brief description of the BFACF algorithm (for details, see ref. 7, Section 3.1). It generates SAWs of variable length  $N$  which begin at the origin and end at a fixed lattice site  $x \neq 0$ ; the elementary moves are local deformations of the chain with  $\Delta N = 0, \pm 2$ . It satisfies detailed balance with respect to a modified canonical ensemble in which each  $N$ -step walk gets relative weight  $N\beta^N$ , where  $\beta$  satisfies  $0 < \beta < \beta_c \equiv 1/\mu$  and  $\mu$  is the connective constant of the lattice. The algorithm is known to be ergodic in  $d=2$ <sup>(8)</sup>; it is nonergodic in  $d=3$  if  $|x|_\infty \equiv \max(|x_1|, |x_2|, |x_3|) = 1$ , because of knotted configurations which cannot be untied. In all other cases the problem of ergodicity is still open.

The dynamical behavior of the BFACF algorithm is rather peculiar. To clarify this point, let us define more precisely what we mean by *autocorrelation time*. Let  $A$  be an observable and let

$$\rho_{AA}(t) = \frac{\langle A(0)A(t) \rangle - \langle A(0) \rangle^2}{\langle A(0)^2 \rangle - \langle A(0) \rangle^2} \quad (2)$$

be its normalized time-autocorrelation function in the stationary stochastic process (i.e., *in equilibrium*). Typically,  $\rho_{AA}(t)$  decays exponentially for large  $t$ , and thus it is natural to define the *exponential autocorrelation time*

$$\tau_{\text{exp},A} = \limsup_{t \rightarrow \infty} \frac{t}{-\log |\rho_{AA}(t)|} \quad (3)$$

and

$$\tau_{\text{exp}} = \sup_A \tau_{\text{exp},A} \quad (4)$$

where the supremum is taken over all observables  $A$  with finite second moment.  $\tau_{\text{exp}}$  controls the “worst-case” rate of convergence to equilibrium; in practical terms it places an upper bound on the number of iterations which must be discarded at the beginning of the run. The other quantity of interest is the *integrated autocorrelation time*

$$\tau_{\text{int},A} = \frac{1}{2} \sum_{t=-\infty}^{\infty} \rho_{AA}(t) \quad (5)$$

which controls the statistical error in the Monte Carlo measurements of  $\langle A \rangle$ . Indeed, the variance of the sample mean  $\bar{A}$  is given by

$$\text{var}(\bar{A}) \approx \frac{1}{n} (2\tau_{\text{int},A}) [\langle A^2 \rangle - \langle A \rangle^2] \quad (6)$$

where  $n$  is the number of measurements.

For the BFACF algorithm, Sokal and Thomas<sup>(9)</sup> have proven the surprising result that  $\tau_{\text{exp}} = \infty$  for all  $\beta > 0$ . This means that for most

observables  $A$  the autocorrelation function  $\rho_{AA}(t)$  decays nonexponentially as  $t \rightarrow \infty$ . However, there is nothing to prevent  $\tau_{\text{int},A}$  from being finite, and indeed one expects  $\tau_{\text{int},A} < \infty$  for reasonable observables  $A$ , i.e., those that are not too strongly coupled to very long walks. It then makes sense to study the dynamic critical exponent  $p_A$  defined as  $\tau_{\text{int},A} \sim \langle N \rangle^{p_A}$  for  $\beta \uparrow \beta_c$ .

For fixed- $N$  algorithms using local deformations (i.e.,  $\Delta N = 0$  only), it can be argued heuristically that  $p \approx 2 + 2\nu$ .<sup>(10)</sup> This estimate is based on considering the motion of the center-of-mass vector of the chain. Roughly speaking, the center-of-mass vector executes a random walk, moving a distance of order  $1/N$  at each elementary move. An “essentially new” configuration is reached when this point has moved a distance of order  $\xi \equiv \langle R_g^2 \rangle^{1/2} \sim N^\nu$  (here  $R_g$  is the radius of gyration of the chain). For this to occur it takes about  $(N\xi)^2 \sim N^{2+2\nu}$  elementary moves. This argument can also be converted into a rigorous proof of the *lower bound*  $p_A \geq 2 + 2\nu$ , where  $A$  is the center-of-mass vector of the chain (ref. 7, Example 3 after Theorem A.7).

This reasoning does not, however, apply to the BFACF algorithm, because the  $\Delta N = \pm 2$  moves cause the center-of-mass vector to move a distance of order  $\xi/N \sim N^{\nu-1} \gg 1/N$ ; indeed, applying the same argument would give  $p \approx 2$ . Moreover, all these arguments are based on the hypothesis that the center-of-mass motion plays the role of the slowest-relaxing mode. However, the results of Sokal and Thomas<sup>(9)</sup> suggest another cause of the slow relaxation of the BFACF algorithm.

Consider for a given walk  $\omega$  the minimum surface area  $\mathcal{A}(\omega)$  spanned by the union of  $\omega$  and  $\omega'$ , where  $\omega'$  is a fixed walk from the origin to  $x$ . The Sokal–Thomas proof that  $\tau_{\text{exp}} = +\infty$  is based on showing that the BCACF algorithm has very slowly relaxing modes associated with transitions to very long walks whose surface area is much greater than their length. Using this same idea, one can also prove (ref. 7, Example 1 after Theorem A.7) that

$$\tau_{\text{int},\mathcal{A}} \geq \text{const} \times [\langle \mathcal{A}^2 \rangle - \langle \mathcal{A} \rangle^2] \tag{7}$$

Assuming the usual scaling behavior  $\mathcal{A} \sim \xi^2$ ,<sup>(11–16),4</sup> this implies

$$\tau_{\text{int},\mathcal{A}} \gtrsim \xi^4 \sim \langle N \rangle^{4\nu} \sim \begin{cases} \langle N \rangle^3 & \text{for } d=2 \\ \langle N \rangle^{\approx 2.35} & \text{for } d=3 \\ \langle N \rangle^2 (\log \langle N \rangle)^{1/2} & \text{for } d=4 \\ \langle N \rangle^2 & \text{for } d \geq 4 \end{cases} \tag{8}$$

<sup>4</sup>In *two dimensions* this scaling behavior seems to be well established both theoretically<sup>(12,13)</sup> and numerically,<sup>(11,14–16)</sup> but we are not aware of any theoretical or numerical work in higher dimensions. Indeed, it seems to be a rather difficult computational-geometry problem to devise an efficient algorithm for computing the minimum surface area spanned by a self-avoiding polygon in dimension  $d \geq 3$ .

and hence  $p_{sc} \geq 4\nu$ . In the absence of any additional physical mechanism for slow modes, it is reasonable to expect that this bound is close to sharp. It is also reasonable to expect that other “natural” observables, such as the chain length  $N$ , should have the same dynamic critical exponent  $p = 4\nu$ .

In a previous paper<sup>(10)</sup> we performed an extensive Monte Carlo simulation of the BFACF algorithm for both SAWs and nonreversal random walks (NRRWs) in two dimensions, obtaining

$$p_A = \begin{cases} 3.0 \pm 0.4 & \text{for } d=2 \text{ SAW} \\ 2.2 \pm 0.5 & \text{for } d=2 \text{ NRRW} \end{cases} \quad (9)$$

(95% subjective confidence limits) for  $A = N$ ,  $N^2$ ,  $N^3$ . This rules out the relation  $p = 2 + 2\nu = 3.5$  (SAW), 3.0 (NRRW), but is consistent with  $p = 4\nu = 3.0$  (SAW), 2.0 (NRRW).

In the present work we augment the previous data in two ways: for the two-dimensional SAW, we have added an additional point at  $\beta = 0.3771$ , closer to criticality; and we have now studied also SAWs in three and four dimensions.

In Tables I–III we report the parameters of our runs and the estimated values of  $\langle N \rangle$  and  $\tau_{\text{int},N}$ . In all cases we chose the endpoint  $x$  to be a nearest neighbor of the origin.<sup>5</sup> We have analyzed the data using standard procedures of statistical time-series analysis, following ref. 21, Appendix C. We have used in all cases a self-consistent rectangular window of width  $10\tau_{\text{int},N}$ .

<sup>5</sup> For  $d = 3$ , the algorithm is nonergodic for this choice of  $x$ , because of knotted configurations which cannot be untied. However, in a separate study<sup>(20)</sup> using the BFACF algorithm combined with 2-pivot cut-and-paste moves<sup>(7)</sup>—an algorithm which *is* ergodic—we found that for  $N \lesssim 200$ , less than 0.1% of the configurations are knotted. So the effects of knots are probably negligible in the simulations reported here.

**Table I. Parameters and Results of Our Runs for  $d = 2^a$**

$\beta$	$\langle N \rangle$	Data-taking interval	run length	$\tau_{\text{int},N}$
0.3690	21.5	7000	$3.5 \times 10^9 \approx 60000\tau_{\text{int},N}$	$56800 \pm 1000$
0.3728	33.6	17000	$8.5 \times 10^9 \approx 40000\tau_{\text{int},N}$	$227000 \pm 8000$
0.3744	44.4	22000	$1.65 \times 10^{10} \approx 35000\tau_{\text{int},N}$	$470000 \pm 17000$
0.3760	72.8	140000	$3.5 \times 10^{10} \approx 20000\tau_{\text{int},N}$	$1940000 \pm 90000$
0.3771	103.0	1000000	$2.0 \times 10^{10} \approx 3000\tau_{\text{int},N}$	$6240000 \pm 700000$

<sup>a</sup> Errors are  $\pm$  one standard deviation. Errors on  $\langle N \rangle$  are less than 3%. Note that  $\beta_c \approx 0.379052$ .<sup>(17)</sup>

**Table II. Parameters and Results of Our Runs for  $d=3^a$**

$\beta$	$\langle N \rangle$	Data-taking interval	Run length	$\tau_{int,N}$
0.2110	33.5	1000	$2.3 \times 10^9 \approx 15000\tau_{int,N}$	$154000 \pm 8000$
0.2115	41.2	5000	$3.0 \times 10^9 \approx 7000\tau_{int,N}$	$459000 \pm 36000$
0.2120	52.1	10000	$7.0 \times 10^9 \approx 12000\tau_{int,N}$	$570000 \pm 33000$
0.2125	72.8	100000	$1.3 \times 10^{10} \approx 10000\tau_{int,N}$	$1346000 \pm 90000$
0.2130	123.8	150000	$1.0 \times 10^{10} \approx 2000\tau_{int,N}$	$4497000 \pm 600000$
0.2132	221.2	200000	$4.5 \times 10^{10} \approx 3000\tau_{int,N}$	$16128000 \pm 1900000$

<sup>a</sup> Errors are  $\pm$  one standard deviation. Errors on  $\langle N \rangle$  are less than 3%. Note that  $\beta_c \approx 0.2135$ .<sup>(18)</sup>

The next step is to estimate the dynamic critical exponent  $p$ , using a weighted least-squares fit to the relation

$$\log \tau_{int,N} = a + p \log \langle N \rangle \tag{10}$$

(In this fit we neglect the error bars on  $\langle N \rangle$ , which are small compared to those on  $\tau_{int,N}$ .) Unfortunately, this analysis is somewhat subtle, due to corrections to scaling: especially for  $d=3, 4$  there is substantial curvature in a log-log plot, when  $\langle N \rangle \lesssim 30-40$ . We therefore performed, for each dimension, a sequence of least-squares fits in which only those data points having  $\beta \geq \beta_{min}$  are included in the fit. The results of this analysis are shown in Table IV. The error bars on  $p$  and  $a$  are one standard deviation, computed using the raw-data error bars from Tables I–III (ref. 22, Chapter 3). The  $\chi^2$  value can then be used as a test of goodness-of-fit.

**Table III. Parameters and Results of Our Runs for  $d=4^a$**

$\beta$	$\langle N \rangle$	Data-taking interval	Run length	$\tau_{int,N}$
0.1465	26.0	12000	$2.28 \times 10^9 \approx 10000\tau_{int,N}$	$228588 \pm 14500$
0.1470	43.4	30000	$9.60 \times 10^9 \approx 6000\tau_{int,N}$	$1548600 \pm 124000$
0.1473	67.3	100000	$3.36 \times 10^{10} \approx 8000\tau_{int,N}$	$3961000 \pm 272000$
0.1475	106.1	400000	$8.00 \times 10^{10} \approx 6000\tau_{int,N}$	$14156000 \pm 1200000$
0.1476	311.4	800000	$6.60 \times 10^{10} \approx 1000\tau_{int,N}$	$78344000 \pm 17000000$

<sup>a</sup> Errors are  $\pm$  one standard deviation. Errors on  $\langle N \rangle$  are less than 7%. Note that  $\beta_c \approx 0.1477$ .<sup>(19)</sup>

Table IV. Results of Least-Squares Fits to the Power-Law Ansatz (10)<sup>a</sup>

$d$	$\beta_{\min}$	$p$	$a$	$\chi^2$
2	0.3690	$2.93 \pm 0.03$	$1.97 \pm 0.11$	6.36 (3 d.f., level = 10%)
2	0.3728	$2.84 \pm 0.07$	$2.33 \pm 0.25$	3.88 (2 d.f., level = 14%)
2	0.3744	$2.95 \pm 0.10$	$1.86 \pm 0.40$	1.55 (1 d.f., level = 21%)
3	0.2110	$2.46 \pm 0.06$	$3.49 \pm 0.23$	42.29 (4 d.f., level = $10^{-8}$ )
3	0.2115	$2.20 \pm 0.07$	$4.68 \pm 0.31$	9.78 (3 d.f., level = 2%)
3	0.2120	$2.32 \pm 0.09$	$4.10 \pm 0.37$	1.06 (2 d.f., level = 59%)
3	0.2125	$2.24 \pm 0.12$	$4.52 \pm 0.55$	0.02 (1 d.f., level = 89%)
4	0.1465	$2.71 \pm 0.06$	$3.73 \pm 0.24$	54.61 (3 d.f., level = $8 \times 10^{-12}$ )
4	0.1470	$2.21 \pm 0.10$	$5.95 \pm 0.41$	11.40 (2 d.f., level = 0.3%)
4	0.1473	$2.15 \pm 0.14$	$6.26 \pm 0.61$	10.94 (1 d.f., level = 0.1%)

<sup>a</sup> Errors are  $\pm$  one standard deviation. Significance level is the probability that  $\chi^2$  exceeds the observed value.

For  $d=2$ , the goodness-of-fit is acceptable (though not great); it gets slightly better if the lowest one or two points ( $\langle N \rangle \approx 21, 34$ ) are dropped. The estimate  $p = 2.93 \pm 0.03$  is only slightly lower than the predicted lower bound  $p \geq 4\nu = 3$ . Indeed, if one believes the lower bound  $p \geq 4\nu$ , then our numerical result is strong evidence that this lower bound is *sharp* (or close to sharp), i.e., that  $p$  is *equal* (or almost equal) to  $4\nu$ .

For  $d=3$ , the goodness-of-fit is acceptable only if the lowest two points ( $\langle N \rangle \approx 33, 41$ ) are dropped.<sup>6</sup> The resulting estimate  $p = 2.32 \pm 0.09$  is in excellent agreement with the predicted lower bound  $p \geq 4\nu \approx 2.35$ , and indeed with the equality  $p = 4\nu$ .

For  $d=4$ , the estimates of  $p$  decrease toward 2 as  $\beta_{\min}$  is increased, but it is impossible to get a reasonable goodness-of-fit no matter how many points are dropped. Indeed, one can foresee that in dimension  $d=4$  the Ansatz (10) should be corrected by a log-log term, as logarithmic violations of simple power-law scaling are expected in view of (8). We therefore tried also a fit to the expression

$$\log \tau_{\text{int}, N} = a + 2 \log \langle N \rangle + q \log \log \langle N \rangle \quad (11)$$

<sup>6</sup> It is plausible that as the dimension  $d$  increases, a larger  $N$  is needed in order for the walk to “explore” adequately the  $d$ -dimensional space: at smaller values of  $N$ , the walk acts as if it lives primarily in a lower-dimensional subspace. This reasoning might explain also the sign of the observed deviation from pure power-law behavior: the estimated  $p$  for  $d=3$  with  $\beta_{\min} = 0.2110$  is shifted toward the  $d=2$  value. The same sign of deviation occurs for the  $d=4$  data discussed below.

The results are shown in Table V. Unfortunately, the goodness-of-fit is as poor here as for a simple power-law fit. Apparently, very strong corrections to scaling are present, and neither a simple power-law form nor a simple logarithmic form is a satisfactory approximation in the range  $50 \lesssim \langle N \rangle \lesssim 300$ . Indeed, on theoretical grounds<sup>(23-25)</sup> one can expect corrections of the form  $\log \log \langle N \rangle / \log \langle N \rangle$ ,  $1/\log \langle N \rangle$ , and so forth. So it is hardly surprising that we are unable to verify the conjectured behavior  $\tau_{\text{int},N} \sim \langle N \rangle^2 (\log \langle N \rangle)^{1/2}$ . In fact, we believe that it is *impossible* to distinguish numerically, at any feasible value of  $\langle N \rangle$ , between a logarithm and a small power. We conjecture that the logarithmic form is the correct one (quite possibly with  $q=1/2$ ), but this will have to be established by theoretical rather than numerical means. All we can say, on the basis of our present data, is that  $\tau_{\text{int},N}$  grows a little bit faster than  $\langle N \rangle^2$ .

In conclusion, our simulation results give strong (but not unequivocal) support to the conjecture that

$$p = 4\nu \tag{12}$$

i.e., that the surface area is indeed the slowest mode of the BFACF dynamics.

Let us remark, finally, that we expect analogous results to be true for the Sterling-Greensite<sup>(26,27)</sup> algorithm for self-avoiding random surfaces (or alternatively for random surfaces without spikes<sup>(28)</sup>) with fixed boundary  $B$ , in a lattice of dimension  $d \geq 3$ . Indeed, let  $\mathcal{V}(S)$  be the minimum three-dimensional volume spanned by the union of  $S$  and  $S'$ , where  $S'$  is a fixed surface with boundary  $B$ . Then one can easily prove the analogue of (7), namely

$$\tau_{\text{int},\mathcal{V}} \geq \text{const} \times [\langle \mathcal{V}^2 \rangle - \langle \mathcal{V} \rangle^2] \tag{13}$$

and it is reasonable to expect that this bound is almost sharp. What is less clear, however, is the correct scaling behavior for  $\langle \mathcal{V} \rangle$  and  $\langle \mathcal{V}^2 \rangle$ . By

**Table V. Results of Least-Squares Fits of  $d = 4$  Data to the Logarithmic Ansatz (11)<sup>a</sup>**

$\beta_{\text{min}}$	$q$	$a$	$\chi^2$
0.1465	$2.99 \pm 0.24$	$2.46 \pm 0.33$	41.18 (3 d.f., level = $6 \times 10^{-9}$ )
0.1470	$1.01 \pm 0.43$	$5.38 \pm 0.62$	10.65 (2 d.f., level = 0.5%)
0.1473	$0.82 \pm 0.65$	$5.68 \pm 0.98$	10.49 (1 d.f., level = 0.1%)

<sup>a</sup> Errors are  $\pm$  one standard deviation. Significance level is the probability that  $\chi^2$  exceeds the observed value.

analogy with walks, one might expect  $\mathcal{V} \sim \xi^3 \sim N^{3\nu_{RS}}$ , where  $N$  is the number of plaquettes in the surface; but this *cannot* be correct if  $\nu_{RS} < 1/3$ , since it is easily seen on geometric grounds that  $\mathcal{V}(S) \geq \text{const} \times N(S)$ . In particular,  $\mathcal{V} \sim \xi^3$  cannot be true in dimension  $d > 8$ , where self-avoiding surfaces are believed<sup>(29)</sup> to have critical exponent  $\nu_{RS} = 1/4$  (just as for branched polymers); nor can it be true in dimension slightly less than 8, where  $\nu_{RS}$  should be given by an expansion in  $\varepsilon = 8 - d$ . Our best guess for what happens is the following:

- (a) In dimension  $d > 8$ , random surfaces degenerate to *shrunk* tubes (i.e., width of order 1) surrounding a treelike branched polymer having  $\sim N$  links. Therefore,  $\nu_{RS} = \nu_{BP} = 1/4$  and  $\mathcal{V} \sim N$ .
- (b) In dimension  $d < 8$ , random surfaces become *inflated* tubes (i.e., width of order  $N^\kappa$  with  $0 < \kappa < \nu_{BP}$ ) surrounding a treelike branched polymer having  $\sim N^{1-\kappa}$  links. Then  $\nu_{RS} = \nu_{BP} > 1/4$ ,<sup>(27)</sup> but  $\mathcal{V} \sim N^{1+\kappa} \gg N$ .

The distinction between these two cases corresponds to the “breathing transition” studied by several authors.<sup>(29–31)</sup> If this is the correct scenario, then statements to the effect that “self-avoiding random surfaces are in the universality class of branched polymers” must be interpreted with caution: branched polymers would describe correctly the *linear size* of random surfaces, but not (in  $d < 8$ ) their *volume*.

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