Improved Algorithms for Simulating Crystalline Membranes

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Abstract

The physics of crystalline membranes, i.e. fixed-connectivity surfaces embedded in three dimensions and with an extrinsic curvature term, is very rich and of great theoretical interest. To understand their behavior, numerical simulations are commonly used. Unfortunately, traditional Monte Carlo algorithms suffer from very long auto-correlations and critical slowing down in the more interesting phases of the model. In this paper we study the performance of improved Monte Carlo algorithms for simulating crystalline membrane, such as hybrid overrelaxation and unigrid methods, and compare their performance to the more traditional Metropolis algorithm. We find that although the overrelaxation algorithm does not reduce the critical slowing down, it gives an overall gain of a factor 15 over the Metropolis algorithm. The unigrid algorithm does, on the other hand, reduce the critical slowing down exponent to $z \approx 1.7$.

1 Introduction

When using Monte Carlo methods to study physical systems one is usually faced with the problem of critical slowing-down (CSD) in the critical region were a typical correlation length of the system diverges. That is, the auto-correlation time of traditional Monte Carlo algorithms, the time it takes to generate “statistically independent” configurations, grows rapidly with system size. For example, for the well known Metropolis and heat-bath algorithms this time grows linearly with the system size, making simulations of large systems prohibitively time consuming.

It is thus very important to construct new Monte Carlo algorithms that can reduce CSD. Much progress has been made in this direction; examples of improved

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algorithms are, to name a few: Adler’s overrelaxation \cite{1}, Fourier acceleration \cite{2},
multigrid \cite{3} and cluster algorithms \cite{4}. Those algorithms have been applied success-
fully to variety of models and, in some special cases, have eliminated CSD altogether. This,
though, is usually accomplished only for relatively simple models, such as free
field theories or spin models with simple interactions. For more complicated models,
where sophisticated methods are harder to implement, the improvement is usually
somewhat less.

In this paper we study the performance of two such improved algorithms,
overrelaxation and multigrid, in simulations of \textit{crystalline membranes}. Crystalline
membranes are internally rigid surfaces, embedded in three dimensions, with an ex-
trinsic curvature term. They exhibit a phase transition between a high-temperature
crumpled and a low-temperature flat phase. It is especially in the flat phase, and at
the \textit{crumpling} transition, that Monte Carlo simulations with traditional algorithms
suffer from very long auto-correlations.

As with many interesting models, the Hamiltonian of a crystalline membrane
is too complicated for a direct implementation of the methods we want to employ.
Some simplifications have to be made. For the overrelaxation we use a quadratic
approximation to the Hamiltonian when choosing a new trial position — this requires
an additional accept-reject step to restore detail balance. This is usually referred to
as \textit{hybrid} overrelaxation. Instead of multigrid we use a simpler implementation, the
\textit{unigrid} algorithm, in which a coarsening transformation of the field configuration is
not needed — the fields at the original (fine) lattice are simulated at all levels.

In addition to the performance of the algorithms, we also examine the impor-
tance of randomness in the updating procedure, i.e. the order in which the fields
are updated. According to standard folklore, too much randomness in the updating
procedure increases CSD as the system takes a drunkard’s walk through the phase
space. Too little noise, on the other hand, increases CSD as well since the system is
too weakly ergodic. It is thus important to tune the amount of randomness in the
algorithm appropriately.

The paper is organized as follows. In Section 2 we describe the particular
model of a crystalline membrane we study, discuss the problems of the simulations
and the performance of the Metropolis algorithm. In Section 3 we describe the
hybrid overrelaxation algorithm and our approximation. In Section 4 we test the
performance of the unigrid algorithm. Finally, in the Section 5, we compare the
overall performance and merits of those different methods and comment on possible
further improvements and applications.

2 A model of crystalline membranes

The model we simulate is a simple discretization of a phantom (non self-avoiding)
crystalline membrane, inspired by the Polyakov action for Euclidean strings with
extrinsic curvature \cite{5,6}. A discrete crystalline membrane is described by a reg-
ular two-dimensional triangulation embedded in three-dimensional space where it is allowed to fluctuate. The Hamiltonian is composed of two terms: a pair potential between neighboring nodes and a bending energy term. As a pair potential we use a simple Gaussian spring potential, and we model the bending energy by a ferromagnetic interaction between neighboring normals to the faces of the surface:

$$\mathcal{H} = \sum_{ij} |\vec{r}_i - \vec{r}_j|^2 + \kappa \sum_{ab} (1 - \vec{n}_a \cdot \vec{n}_b).$$

Here $i, j$ label the intrinsic position of the nodes, $\vec{r}_i$ is the corresponding position in the embedding space, $\vec{n}_a$ is a normal to a triangle $a$, and $\kappa$ is the bending rigidity.

The partition function is given by the trace of the Boltzmann weight over all possible configurations of the embedding variables $\{\vec{r}\}$:

$$Z = \int [d\vec{r}] \delta(\vec{r}_{cm}) \exp\left(-\mathcal{H}[\vec{r}]\right).$$

The center of mass of the membrane, $\vec{r}_{cm}$, is kept fixed to eliminate the translational zero mode. As there is no self-avoidance term in the Hamiltonian, this model describes a phantom surface.

This model has been studied extensively with numerical methods. It has been found to have a high-temperature crumpled (disordered) phase and a low-temperature flat (ordered) phase, separated by a continuous phase transition — the crumpling transition. The behavior of the system in the flat phase is governed by an infrared stable fixed point at $\kappa = \infty$; the whole flat phase is critical. The existence of an ordered phase in a two-dimensional system with a continuous symmetry and short range interactions is remarkable, given the Mermin-Wagner theorem. What stabilizes the flat phase are the out-of-plane fluctuation of the membrane that couple to the in-plane phonon degrees of freedom due to non-vanishing elastic moduli. Bending of the membrane is necessarily accompanied by an internal stretching. By integrating out the phonon degrees of freedom, one is left with an effective Hamiltonian with long-range interactions between the Gaussian curvature fluctuations.

Most numerical simulations so far have used either local updating methods, usually the Metropolis algorithm, or Fourier acceleration. The Metropolis algorithm, apart from suffering from CSD, has very long auto-correlations both in the flat phase and close to the crumpling transition. To establish this we have simulated the model Eq. (2), using the Metropolis algorithm, on a $L \times L$ square lattice, $L$ ranging from 8 to 64, and with periodic boundary conditions. We choose to simulate the model in the flat phase, at $\kappa = 1.1$, were we know from previous simulations that the auto-correlation time is indeed very long.

To estimate the auto-correlations we measure the square radius of gyration:

$$R_g = \left\langle \sum_i \vec{r}_i \cdot \vec{r}_i \right\rangle.$$
Table 1: The integrated auto-correlation time $\tau$ (in number of sweeps), together with the CPU-time per sweep $T_s$ (in ms). Column (a) is for a lexicographic update of nodes, while (b) is for random updating. From a linear fit to Eqs. (6) and (7) we get the exponents $z_a$ and $z_s$ and the corresponding amplitudes $A_a$ and $A_s$.

| L  | $\tau$ (a) | $T_s$ (a) | $\tau$ (b) | $T_s$ (b) |
|----|------------|----------|------------|----------|
| 8  | 219(15)    | 1.112    | 227(12)    | 1.036    |
| 12 | 546(35)    | 2.784    | 567(30)    | 2.610    |
| 16 | 1153(90)   | 4.900    | 1123(80)   | 4.688    |
| 24 | 2714(150)  | 10.86    | 2534(220)  | 11.01    |
| 32 | 4049(210)  | 22.23    | 4527(260)  | 21.68    |
| 48 | 11443(600)| 52.33    | 10347(550)| 50.60    |
| 64 | 20500(1200)| 97.59    | 19900(1300)| 98.18    |

As an estimate of CSD we define the dynamical critical exponent $z_a$ using finite size scaling:

$$\tau \approx A_a \xi^{z_a}. \quad (6)$$

i.e. the linear extent of the membrane in the embedding space. This is usually the “slowest mode” of the system. From this we construct the normalized auto-correlation function

$$\rho(s) = \frac{\langle R_g(t+s)R_g(t) \rangle - \langle R_g \rangle^2}{\langle R_g^2 \rangle - \langle R_g \rangle^2}, \quad (4)$$

and the integrated auto-correlation time (measured in units of sweeps)

$$\tau = \frac{1}{2} + \sum_{s=1}^{\infty} \rho(s). \quad (5)$$

This is shown in Table 1. The errors on the auto-correlation times are estimated from 10 to 20 independent runs, each few hundred $\tau$ long.

As mentioned in the introduction, we also want to understand the effect of randomness in the updating on performance. Thus we have repeated the simulations for two different updating schemes: the nodes are sampled either at random or they are traversed in a lexicographic order. Lexicographic order means that the node at (intrinsic) position $\vec{x}$ is always updated before $\vec{x} + \vec{e}_i$ ($i = 1, 2$), except at the boundaries. For a free field theory, updated with the overrelaxation algorithm, only the latter scheme reduces CSD [10].
Here $\xi$ is some characteristic length scale of the system; in our simulations, where the model is critical, this is the intrinsic linear extent $L$.

To evaluate the performance of the algorithm, we also have to take into account the amplitude $A_a$ and how the computational work performed per sweep, measured in CPU-time $T_s$, scales with system size. This we include in Table 1. Similarly to Eq. (6) we define an exponent $z_s$:

$$T_s \approx A_s t^{z_s},$$

where $t$ is now measured in “real” time (in ms). Combining these exponents and amplitudes, the performance — the total “cost” of the algorithm — is given by $T = A_s A_a t^{z_a + z_s}$. For the Metropolis algorithm we get:

$$T_M = \begin{cases} 0.0332(45) L^{4.304(57)} & \text{lexicographic updates}, \\ 0.0314(48) L^{4.316(67)} & \text{random updates}. \end{cases}$$

For this algorithm, the order in which nodes are updated is irrelevant.

### 3 Hybrid overrelaxation

Overrelaxation was introduced as a generalization of the heat-bath algorithm for models with multi-quadratic actions [1]. In the original formulation the new value of a field $\phi_i$ is chosen to be negatively correlated with the old value. Given a multi-quadratic action,

$$S = \omega (\phi_i - \mathcal{F}_i[\phi_{j\neq i}])^2 + \{ \text{terms independent of } \phi_i \}, \quad (9)$$

one chooses a local update of the field $\phi_i$ as

$$\phi_i \rightarrow \phi'_i = (1 - \zeta)\phi_i + \frac{\zeta}{\omega^2} \mathcal{F}_i + \frac{\sqrt{\zeta(2 - \zeta)}}{\omega} \xi. \quad (10)$$

$\xi$ is a Gaussian random variable of unit variance and $\zeta$ is a relaxation parameter. This update fulfills detail balance for $0 < \zeta \leq 2$; for $\zeta = 1$ it reduces to the standard heat-bath algorithm, while for $\zeta = 2$ the field evolution becomes deterministic and conserves energy (a micro-canonical simulation). In the latter case, in order to restore ergodicity, some amount of standard ergodic updates have to be included.

This method has been applied successfully to variety of models; its success based on it suppressing the usual random walk behavior of local updating algorithms [11]. In order to achieve the greatest reduction of CSD, both the relaxation parameter $\zeta$, and the noise in the updating procedure, should be fine-tuned [10, 14]. Unfortunately, the usefulness of the method has been limited by its restriction to multi-quadratic systems.
A number of generalizations of the overrelaxation have been proposed [12]. They usually involve a transformation of the Boltzmann distribution to the appropriate form Eq. (9), and the introduction of an accept-reject step to ensure detail balance. This has the disadvantage that the accept-reject step can enhance random walk behavior by the algorithm and, in addition, the rejection probability usually depends on some characteristics of the model and may not be adjustable to a reasonable value. This is nevertheless the approach we will use.

We make a quadratic approximation to the Hamiltonian Eq. (1) and then apply hybrid overrelaxation (with \( \zeta = 2 \)). We treat the non-linear bending energy term by assuming that normalization in the denominator is constant for all the triangles, i.e. we write the normals as

\[
\vec{n}_a(\vec{r}) = \frac{(\vec{r}_i - \vec{r}_j) \times (\vec{r}_i - \vec{r}_k)}{\sqrt{|(\vec{r}_i - \vec{r}_j) \times (\vec{r}_i - \vec{r}_k)|^2}} \approx \frac{\vec{r}_j \times \vec{r}_k - \vec{r}_i \times (\vec{r}_j + \vec{r}_k)}{\Lambda}, \tag{11}
\]

were \( \{i, j, k\} \) are the nodes defining triangle \( a \). Then, a quadratic approximation to the Hamiltonian can be written as

\[
\mathcal{H}_A = \sum_{\langle ij \rangle} (\vec{r}_i - \vec{r}_j)^2 - \frac{\kappa}{\Lambda^2} \sum_{\langle ab \rangle} [\vec{r}_j \times \vec{r}_k - \vec{r}_i \times (\vec{r}_j + \vec{r}_k)] \cdot [\vec{r}_k \times \vec{r}_i - \vec{r}_i \times (\vec{r}_k + \vec{r}_i)], \tag{12}
\]

where the triangles \( a = (i, j, k) \) and \( b = (i, k, l) \) are adjacent. Since the approximate Hamiltonian is quadratic in \( \vec{r}_i \), we can write:

\[
\mathcal{H}_A = \vec{r}_i \cdot (\hat{M} \vec{r}_i) + \vec{C} \cdot \vec{r}_i + \{\text{terms independent of } \vec{r}_i\}. \tag{13}
\]

The matrix \( \hat{M} \) and the vector \( \vec{C} \) are easily computed:

\[
\hat{M}_{aa} = 6 - \frac{\kappa}{\Lambda^2} \sum_{j=1}^{6} \sum_{b \neq a} \left( r_j^{(b)} - r_j^{(b)} \right) \left( r_{j+1}^{(b)} - r_j^{(b)} \right),
\]

\[
\hat{M}_{a \neq b} = \frac{\kappa}{\Lambda^2} \sum_{j=1}^{6} \left( r_j^{(a)} - r_j^{(a)} \right) \left( r_{j+1}^{(b)} - r_j^{(b)} \right), \tag{14}
\]

and

\[
C^{(a)} = -\sum_{j=1}^{6} \left\{ r_j^{(a)} \left[ \frac{\kappa}{\Lambda^2} \left( r_j \cdot (2\vec{r}_{j-1} + 2\vec{r}_{j+1} - \vec{q}_j - \vec{q}_{j-1}) - (\vec{r}_{j+1} + \vec{r}_{j-1})^2 
+ \vec{r}_{j-1} \cdot \vec{r}_{j-2} + \vec{r}_{j+1} \cdot \vec{r}_{j+2} \right) - 2 \right] + \frac{\kappa}{\Lambda^2} q_j^{(a)} (\vec{r}_{j+1} - \vec{r}_j)^2 \right\}. \tag{15}
\]

The indices \( a \) and \( b \) label the component of the fields in the embedding space, and the index \( j \) labels the neighbors of node \( i \), including its next-to-nearest neighbors \( \vec{q}_j \), in a cyclic manner.
Figure 1: The integrated auto-correlation time $\tau$, vs. the “normalization” parameter $\Lambda$, for the hybrid overrelaxation algorithm. This is shown both for a random (squares) and a lexicographic (circles) updating. The lattice size is $16^2$. The dashed line is the corresponding acceptance rate $\rho$ in the Metropolis test.

The constant energy surface, $H_A(\vec{r}_i) = k$, is a multi-quadratic function — in our case an ellipsoid in the embedding space. To find the new (overrelaxed) embedding position $\vec{r}_i'$, we can diagonalize the matrix $\hat{M}$ and apply overrelaxation to the transformed variables. This involves some amount of calculation; a quicker and sufficient method is to apply overrelaxation in a random sequence to each of the embedding positions $\vec{r}_{i(a)}$, $a = 1, 2, 3$. Once the trial position has been chosen, it is accepted or rejected according to a Metropolis test.

An important feature of this approximation is the parameter $\Lambda$. Although introduced as a substitution for the normalization of the normals, it can be tuned to optimize the performance of the algorithm by minimizing the rejection probability in the Metropolis test.

We have applied this method in the flat phase ($\kappa = 1.1$) for both random and lexicographic updating. To ensure ergodicity we also include a random amount of standard Metropolis updates (about 20%). In Fig. 1 we show the integrated auto-correlation time vs. $\Lambda$, for a lattice size $L = 16$. We also include the corresponding acceptance rate in the Metropolis test. In this case, contrary to the Metropolis algorithm, lexicographic updating reduces $\tau$ by about 30%, independent of system size. More important, for a suitable choice of $\Lambda$, $\tau$ is reduced by a factor of 15 relative to the Metropolis algorithm. As it might be expected, the optimal choice of
Table 2: Same as Table 1, except the algorithm used is the approximate hybrid overrelaxation. Again (a) corresponds to lexicographic and (b) to random updating. The optimal value of the parameter $\Lambda$ is also included.

| $L$ | $\Lambda$ | $\tau$ | $T_{\text{sweep}}$ | $\Lambda$ | $\tau$ | $T_{\text{sweep}}$ |
|-----|--------|------|-------------|--------|------|-------------|
| 8   | 1.08   | 18.5(7)| 1.247      | 1.08   | 31.9(1.2)| 1.136       |
| 12  | 1.23   | 36.6(1.1)| 3.078    | 1.22   | 66.9(2.0)| 2.766       |
| 16  | 1.38   | 70.6(8.0)| 5.735   | 1.35   | 113.3(6.0)| 5.122       |
| 24  | 1.57   | 150(11)| 13.42     | 1.58   | 279(18)  | 11.83       |
| 32  | 1.92   | 269(25)| 27.27     | 1.94   | 484(42)  | 24.12       |
| 48  | 2.68   | 640(40)| 62.69     | 2.60   | 1096(90)| 53.19       |
| 64  | 3.09   | 1120(105)| 118.7   | 3.20   | 2600(180)| 103.5       |
| $z$ | 1.990(31)| 2.190(14) |         | 2.065(30)| 2.163(18) |         |
| $\mathcal{A}$ | 0.275(24) | 0.0132(6) |         | 0.405(34) | 0.0127(8) |         |

$\Lambda$ corresponds to maximizing acceptance rate in the Metropolis test. Surprisingly this value is much higher than one would expect from the average length of the un-normalized normals ($\langle|\vec{n}_{\text{un}}|\rangle \approx 0.3$ for $\kappa = 1.1$). This implies that, in order to enhance the acceptance rate, it is convenient to suppress the bending energy term in the approximation.

We have repeated this analysis for lattices sizes $L = 8$ to 64. In Table 2 we show the optimal values of $\Lambda$, the corresponding integrated auto-correlation time and the CPU-time for a sweep. From this data we extract, as before, the exponents $z_a$ and $z_s$ and the amplitudes $\mathcal{A}_a$ and $\mathcal{A}_s$, and obtain the following performance:

$$
\tau_0 = \begin{cases} 
0.00364(36) & L^{4.167(46)} \quad \text{lexicographic updates,} \\
0.00514(30) & L^{4.228(48)} \quad \text{random updates.}
\end{cases}
$$

Although hybrid overrelaxation does not reduce CSD, it gives an improvement of one order of magnitude over the Metropolis algorithm, provided the nodes are updated in a lexicographic order and the “normalization” parameter $\Lambda$ is properly adjusted.

4 A unigrid Monte Carlo algorithm

The critical slowing down of traditional Monte Carlo algorithms arises mainly from the fact that the update is local, and thus the system takes a random walk through the configuration space. This can be improved by using collective mode (non-local) updating such as multigrid methods [3, 13]. The basic idea is to consider a sequence of coarser lattices (levels) in addition to the original lattice. At each level the system is updated using traditional methods but, as this is repeated recursively at all length scales, the long wavelength modes are equilibrated much faster.
There are several basic ingredients to a multigrid algorithm: a restriction operator and the corresponding interpolation operator, or kernel, are needed to map the system onto the coarser lattices and back; an updating algorithm, such as Metropolis, is applied at each level; finally, one has to choose how to traverse the different levels.

For a crystalline membrane it is not possible to construct an exact interpolation operator between different levels due to the complexity of the Hamiltonian Eq. (1). This problem can be circumvented by using an alternative implementation, the unigrid method, in which the coarse lattices are simply defined as subdivisions of the original one; the update of a coarse lattice acts on blocks of the original fields. For the update, the choice is usually between a piecewise constant or a piecewise linear kernel. A piecewise kernel simply shifts all of the fields in the block by a uniform value. A piecewise linear kernel shifts the fields by a value linearly interpolated between zero, at the boundary, and a maximum value at the center of the block. The shift operation is one of the global symmetries of the system.

Several considerations should be made in choosing a kernel. The piecewise linear kernel has the advantage that the acceptance rate of the proposed moves does not depend on the block size. For a crystalline membrane, on the other hand, this is outweighed by the computational cost which, as all the normal-normal interactions in the block have to be recalculated, grows linearly with the block size. Hence a piecewise constant kernel is preferable, since the sole contribution to the energy change comes from the boundary.

We parameterize a non-local change of the configuration, when we shift a block $\Lambda_k$ at level $k$, as:

$$
\vec{r}_i' = \begin{cases} 
\vec{r}_i + \epsilon_k \vec{x} & \text{if } i \in \Lambda_k \\
\vec{r}_i & \text{otherwise,}
\end{cases}
$$

(17)

where $\vec{x}$ is some normalized random noise and $\epsilon_k$ is the amplitude of the shift. A necessary prerequisite for the unigrid method to be efficient is that the energy cost does not grow too fast with the perimeter $L_k$ of the block. Stated differently: in order to maintain a constant acceptance rate in the Metropolis test, the amplitudes have to be scaled like

$$
\epsilon_k \sim L_k^{-\alpha}.
$$

(18)

If the exponent $\alpha$ is too big, i.e. of order unity, it is unlikely that any multigrid algorithm will reduce CSD.

Following the analysis of [15], we can estimate whether the unigrid update has a chance of improving the dynamical behavior in the case of a crystalline membranes. Assuming that the probability distribution is nearly Gaussian, one can approximate the acceptance rate by

$$
\Omega(\epsilon) \sim \text{erfc}(\sqrt{h}/2),
$$

(19)

where $h = \langle \Delta \mathcal{H} \rangle$ is the average change in energy and $\epsilon$ is the amplitude of the proposed move. For a piecewise constant kernel we take the Hamiltonian Eq. (1),
Table 3: The auto-correlation and CPU-times for the unigrid algorithm. Results are shown both for \( V \) and \( W \)–cycles.

| \( L \) | \( V \)-cycle \( \tau \) | \( T_s \) | \( W \)-cycle \( \tau \) | \( T_s \) |
|------|----------------|-----|----------------|-----|
| 8    | 17.1(0.4)     | 3.123 | 14.0(0.3)     | 4.195 |
| 16   | 45.8(3.2)     | 16.325 | 30.1(0.9)     | 25.904 |
| 32   | 115.2(6.1)    | 107.18 | 51.0(2.1)     | 203.24 |
| 64   | 269.3(19.1)   | 524.70 | 96.8(8.7)     | 1324.25 |
| \( z \) | 1.349(28)     | 2.489(55) | 0.955(27)     | 2.788(45) |
| \( A \) | 1.040(77)     | 0.0175(31) | 3.96(14)     | 0.0123(18) |

insert Eq. (17) and expand the change in the energy in powers of \( \epsilon \):

\[
\langle \Delta \mathcal{H}(\{\vec{r}_i\};\vec{x}) \rangle = \epsilon \langle F_1(\{\vec{r}_i\};\vec{x}) \rangle + \epsilon^2 \langle F_2(\{\vec{r}_i\};\vec{x}) \rangle + \mathcal{O}(\epsilon^3).
\] (20)

The key observation is that under a global sign change, \( \vec{r}_i \rightarrow -\vec{r}_i \ \forall i \), the function \( F_1 \) changes sign (as each term is a product of odd number of fields \( \vec{r}_i \)), hence \( \langle F_1(\{\vec{r}_i\};\vec{x}) \rangle = 0 \). The leading contribution to \( h \) is therefore proportional to \( \epsilon^2 \). At the same time, the number of terms contributing to Eq. (20) depends linearly on the length of the boundary. Therefore, in order to maintain a constant acceptance rate, one should scale the amplitudes as \( \epsilon \sim L_B^{-1/2} \). This agrees with our numerical simulations where we find \( \alpha = 0.52(1) \).

Another free parameter in the unigrid method is the relative frequency with which different levels are updated. One must strike a balance between the effectiveness of block moves and their relative computational cost. Two general schemes are used in the literature; the \( V \) and \( W \)–cycles. In a \( V \)-cycle the levels are updated consecutively, from the finest to the coarsest and back, whereas a \( W \)-cycle recursively applies a \( V \)-cycle at each visited level, spending more time in updating coarser levels. For multigrid algorithms, where the lattices size decreases between levels, a \( W \)-cycle is preferable, provided that the interpolations between levels is not too time consuming. For a unigrid algorithm the computational cost increases with the block size, as discussed above, and, depending on the exponent \( \alpha \), a \( V \) or \( W \)-cycle will be advantageous. For a piecewise constant kernel the computational cost scales like \( L_B \) and a \( W \)-cycle might be advantageous, while for a piecewise linear kernel the computational cost scales linearly with the area of the block and a \( V \)-cycle would be better.

As before, we have simulated a crystalline membrane in the flat phase and for lattice sizes \( L = 8, 16, 32 \) and 64, using the unigrid algorithm and updating the system at each level with the Metropolis algorithm. We repeated the simulation both for a \( V \) and \( W \)-cycle. In Table 3 the measured value of the auto-correlation and CPU-times, from which we determine the overall performance of the
algorithm:

\[
\mathcal{T}_U = \begin{cases} 
0.0182(35) \ L^{3.838(84)} & \text{V-cycle,} \\
0.0242(39) \ L^{3.743(72)} & \text{W-cycyle.}
\end{cases}
\]  

In both cases the unigrid algorithm reduces CSD, albeit not very much, but enough to make it worthwhile for large membranes. For the W–cycle this implies a dynamical CSD exponent \( z \approx 1.7 \), although this value is probably to large, as we observe strong finite size effects in the fit to Eq. (18); if we exclude the smallest volume \((L = 8)\), we get \( z \approx 1.6 \). In conclusion, although the W–cycle is more time consuming per sweep, its performance is better than V–cycle in simulations of membranes of size \( L \gtrsim 20 \).

5 Discussion

Comparing the performance of these different algorithms, Eqs. (8), (16), and (21), we see that, in the simulation of crystalline membranes on realistic lattice sizes \((L = 10 \text{ to } 200)\), both the hybrid overrelaxation and the unigrid algorithm reduce the computational cost by an order of magnitude over the Metropolis algorithm. As the unigrid algorithm also reduces the dynamical exponent \( z \), especially using a W–cycle, it is clearly the best choice for large membranes. In the particular case we studied in this paper, large means \( L \gtrsim 50 \), although this value may depend on the simulation parameters (i.e. \( \kappa \)).

We would also like to emphasize that, in order to achieve optimal performance of the hybrid overrelaxation, it is imperative to adjust the noise in the updating procedure (to use lexicographic updating), and to tune the “normalization” parameter \( \Lambda \) appropriately.

An alternative algorithm used to simulate crystalline membranes is a combination of Langevin updates with Fourier acceleration [7, 8]. This algorithm is known to substantially reduce CSD, although the gain is lost to some extent in the large computational overhead. This method is also complicated by systematic errors induced by using a finite time step \( \Delta t \); this necessitates an extrapolation to \( \Delta t = 0 \), which can itself become time consuming. Nevertheless, it would be interesting to know how well this algorithm performs, in realistic simulations, compared to the algorithms we have studied in this paper. Unfortunately, we do not have an estimate of its performance in similar conditions (e.g., using the same computers) for comparison.

An obvious extension of the methods studied in this paper, is to combine hybrid overrelaxation with the unigrid algorithm. It is possible to maximize the shift of a block in a unigrid update, by choosing it in a deterministic and energy preserving way, improving the performance even further. This is though more complicated to implement and it is under investigation.

There are few application in which the hybrid overrelaxation might be more advantageous compared to the unigrid algorithm. Overrelaxation can be parallelized.
in a straightforward manner, although it could be difficult to define a lexicographic update in that case. It also easy to adapt hybrid overrelaxation to modified versions of the model like, for example, self-avoiding crystalline membranes, which are of great physical interest. In that case, a proposed updated is rejected if it leads to self-intersection of the membrane. Intuitively, a non-local change, like one proposed by the unigrid algorithm, is more likely to be rejected — hybrid overrelaxation might turn out to be more effective.

Finally, we would like to point out that both these updating algorithms can be used in simulations of fluid membranes with extrinsic curvature [16]. In that case, the surface fluctuates in the embedding space, and its connectivity matrix changes dynamically. It is known that simulations of fluid membranes suffer from even longer auto-correlation times than their crystalline counterparts. For fluid membranes, the random nature of the lattice causes some complications in implementing hybrid overrelaxation and unigrid algorithms. For example, it is not obvious how to define lexicographic ordering. A possible method would be to propagate the updates outwards from a randomly chosen node, i.e. by traversing the lattice in steps of increasing geodesic distance from a marked point. For the unigrid algorithm the problem is that a random lattice cannot be divided into regular blocks. Again, blocks could be defined as nodes within a given geodesic distance from some randomly chosen node.

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