Coupling methods for efficient simulation of spatial population dynamics

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Abstract

Coupling is a widely used technique in the theoretical study of interacting stochastic processes. In this paper I present an example demonstrating its usefulness also in the efficient computer simulation of such processes. I first describe a basic coupling technique, applicable to all kinds of processes, which allows trading memory use for a limited speedup. Next, I describe a specialized variant of it, which can be used to speed up the simulation certain kinds of processes satisfying a monotonicity criterion. This special algorithm increases the speed by several orders of magnitude with only a modest increase in memory usage.

Keywords:
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1. Introduction

In its most basic form, coupling means constructing multiple stochastic processes on the same underlying probability space (Liggett, 1999). In a computer simulation, the role of the underlying probability space is played by the random number generator, and the coupling techniques presented in this paper can be described as simulating multiple realizations of a stochastic process in parallel using the same stream of random events.

The processes to which I will apply the simulation techniques described below belong to the class of lattice contact processes introduced by Harris (1974) as models of an endemic infection in a spatially structured host population. While the simulation techniques described in this paper—particularly in section 2—may in principle also be applied to other interacting stochastic processes (like e.g. the Ising process from statistical physics), they were developed with the contact process in mind, and it is the contact process which I will use to demonstrate them here.

In the basic lattice contact process, each site on a regular lattice represents a single host individual, which, at any given time, may be in one of two states: uninfected (0) or infected (1). The state of the lattice, which consists of the states of the individual sites, evolves as a continuous time Markov process. Figure 1 shows a conceptual illustration of the possible local transitions which may occur: each infected site recovers independently with rate \( r \) and transmits the infection to a random neighbor site with rate \( c \).

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The word “neighbor” here should be understood in a broad sense: the algorithms given in this paper work just as well regardless of which sites are considered to be neighbors, and they can even be straightforwardly generalized to handle arbitrary dispersal kernels or contact networks, where different pairs of sites may have different probabilities of infecting each other. Indeed, they can even be adapted to simulate spatio-temporal point processes in continuous space. Also, while I’ve followed the terminology of Harris (1974) in describing the lattice sites as “hosts” which may be “infected” or “uninfected”, they can be more generally interpreted e.g. as occupied or vacant habitat patches in a stochastic patch occupancy model of metapopulation dynamics, or as individual spatial loci in a lattice model of a plant population. In section 4 I also describe an application of these techniques to models with more than one competing infector strain.

Algorithm 1: Naive contact process simulation.

Data: \( S_x \in \{0,1\} \quad \forall x \in L = \{1,\ldots,N\} \)

while \( t < t_{\text{max}} \) do
  \( A := \text{random site in } L \)
  \( x := \text{random number in } [0,r+c) \)
  if \( x < c \) then
    perform a contact event:
    \( B := \text{random neighbor of } A \)
    \( S_B \leftarrow 1 \text{ if } S_A = 1 \)
  else
    perform a recovery event:
    \( S_A \leftarrow 0 \)
  end
  advance clock by mean time between events:
  \( t \leftarrow t + \frac{1}{(r+c)} \)
end

Algorithm 1 shows a straightforward naive (i.e. unoptimized) algorithm for simulating the basic lattice contact process. Here the array \( S \) stores the current state (0 for uninfected, 1 for infected) of each site on the lattice \( L \). At every iteration, a single site \( A \) on the lattice is randomly chosen as the focus of an event, which will be a contact event if the uniform random variable \( x \in [0,r+c) \) is less than \( c \) and a recovery event otherwise. After each iteration, the time \( t \) is advanced by the expected time \( 1/(r+c) \) between events per site, divided by the total number of sites \( N \).

Experienced readers may note that there are several optimizations that could be made to algorithm 1. For example, it is wasteful to sample the focal site \( A \) from the entire lattice \( L \), when we could instead maintain a list of the currently infected sites and sample \( A \) from that list. For simplicity, I will not include such well known optimizations in the example algorithms presented here, nor will I discuss them except where relevant to the methods introduced below.

2. Coupling

A general way to speed up algorithm 1 is to simulate multiple coupled instances of the process in parallel, as shown in algorithm 2.

Here we have \( n \) contact processes with contact and recovery rates \( c_k \) and \( r_k \), \( k \in K = \{1,\ldots,n\} \) respectively, and instead of single states, the array \( S \) contains vectors of \( n \) states \( S_A = (S_{A1}, S_{A2}, \ldots, S_{An}) \) for each site \( A \). The fixed \( r \) and \( c \) from algorithm 1 are replaced with \( r_{\text{max}} = \max_{k \in K} r_k \) and \( c_{\text{max}} = \max_{k \in K} c_k \) respectively, but we update the \( k \)-th element of the state vector on each contact event only if \( x < c_k \), and on each recovery event only if \( x < c_{\text{max}} < r_k \). In this way, the effective contact and recovery rates for the \( k \)-th process remain \( c_k \) and \( r_k \) respectively.

Figure 2 illustrates some example state transitions in algorithm 2. Here the columns of circles represent the state vectors of two neighboring sites.

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2 Strictly speaking, the time between consecutive events should, of course, be an exponentially distributed random variable, but replacing this random variable with its expectation is a commonly used simplification, justified by the fact that the expected difference between the approximate time so obtained and the ‘true’ time scales as \( \sqrt{N(r+c)} \), and thus becomes relatively negligible compared to \( t \) when \( tN(r+c) \gg 1 \) (i.e. after a large number of events).
Whenever a contact or recovery event is performed, the random variable $x$ is used to determine the set of $k$ values for which the event in question actually takes place, with the remaining elements in the state vectors being unchanged.

Of course, the realizations of the processes simulated using algorithm 2 will not be independent, even though it is easy to see that each process has the correct marginal transition probabilities when considered separately from the others. This lack of mutual independence must be kept in mind when interpreting the results. In particular, when sampling the behavior of a model over a range of parameter values using traditional simulation methods like algorithm 1, a fairly common practice is to use only one simulation run for each parameter value and to instead increase the number of parameter values sampled, so that any stochastic variation in the results will hopefully be evident as lack of correlation between nearby sample points. While using algorithm 2 allows the process to be simulated for many parameter values at once, the tradeoff is that any stochastic variation in the results of a single run will be strongly correlated, and so multiple runs will be necessary to properly estimate variances in the results. Even so, the number of runs of algorithm 2 needed to obtain results of comparable quality will often compare favorably with naively sampling the parameter space using algorithm 1.

The performance gains for this basic coupling technique come mainly from the reduction in loop overhead (i.e. the time spent executing the loop-stopping instructions, updating the clock variable, etc.) and random number generator calls. In particular, note that algorithm 2 consumes just as many random numbers to simulate $n$ coupled processes as algorithm 1 needs to simulate just one. Random number generation can be a time-consuming process, particularly if a high quality random number generator is used, and thus the time savings from minimizing random number use can be substantial. Depending on how the array $S$ is stored in memory, the locally sequential memory access pattern of reading and writing one whole state vector at a time may also be more efficient that the completely random pattern in algorithm 1, particularly if a compact representation of the state vectors is used.\footnote{In languages that don’t have a native compactly stored bit vector datatype, vectors of 8, 16, 32 or 64 bits can be stored in suitably sized integer variables. A convenient feature of such a representation is that the inner loops in algorithm 2 can be replaced by bitwise Boolean logic operations such as $S_B \leftarrow S_B \lor (S_A \land M(x))$, where the mask $M(x)$ can be efficiently looked up using e.g. the square histogram method of Marsaglia et al. (2004). For longer vectors, arrays or tuples of integers may be used.}

The down side, of course, is that no matter how compactly the state vectors are represented, each vector of $n$ states needs at least $n$ bits of memory. In particular, the lattice size and the number of coupled processes needs to be kept low enough that the entire lattice fits in the available memory without swapping to disk, or else performance is likely to suffer catastrophically. In practice, some trial and error may be necessary to find the optimal number of coupled processes to maximize overall simulation speed on a given system.

It is also worth noting that the speed of the coupled simulation depends on the maximum rates of each type of event over the coupled processes. If the processes vary widely in their respective event rates, those with rates significantly below the maximum will be simulated less efficiently than they would be on their own, requiring the simulation to be run

\begin{algorithm}
\begin{algorithmic}
\State {Data: $S_{x,k} \in \{0, 1\}$ $\forall x \in L = \{1, \ldots, N\}, k \in K = \{1, \ldots, n\}$}
\State $c_{\text{max}} := \max(c_1, \ldots, c_n)$
\State $r_{\text{max}} := \max(r_1, \ldots, r_n)$
\While {t < $t_{\text{max}}$}
\State $A := \text{random site in } L$
\State $x := \text{random number in } [0, r_{\text{max}} + c_{\text{max}})$
\If {$x < c_{\text{max}}$}
\State $B := \text{random neighbor of } A$
\For {$k \in \{1, \ldots, n\}$}
\If {$x < c_k$ and $S_{A,k} = 1$}
\State $S_{B,k} \leftarrow S_{A,k}$
\EndIf
\EndFor
\Else
\State $\text{perform a recovery event:}$
\For {$k \in \{1, \ldots, n\}$}
\If {$x - c_{\text{max}} < r_k$ then $S_{A,k} \leftarrow 0$}
\EndIf
\EndFor
\EndIf
\State $\text{advance clock by mean time between events:}$
\State $t \leftarrow t + \frac{(r_{\text{max}} + c_{\text{max}})N}{M}$
\EndWhile
\end{algorithmic}
\end{algorithm}
longer. In such cases, it may be more efficient to split the processes into groups with similar event rates and to simulate each group separately. Such grouping is particularly recommended when using optimization techniques, such as those mentioned at the end of section 1, which depend on a substantial fraction of the sites being entirely uninfected or entirely infected.

3. Monotone coupling

In some cases the general coupling technique described above can be made much more efficient yet. In particular, consider what would happen if we could order the coupled processes in algorithm 2 such that $c_i \leq c_j$ and $r_i \geq r_j$ for all $i < j$. Then, if we also chose the initial condition so that, for all $1 \leq A \leq N$ and $i < j$, $S_{A,i} \leq S_{A,j}$, this condition would still hold after one iteration of the main loop, and so would continue to hold after any number of iterations.

Thus, we wouldn’t need to keep track of the entire state vector $S_A$ for each site $A$, but only of the lowest $k$ for which $S_{A,k} = 1$, allowing us to run arbitrarily many coupled processes in parallel with much lower memory usage (about $\log_2 n$ bits of memory per site) than with algorithm 2 (which needs $n$ bits per site).

More generally, let $S_A(p)$ denote the state of the site $A$ at a given time under some family of coupled interacting stochastic processes parametrized by the value $p$. If the initial condition

$$p \leq p' \implies S_A(p) \leq S_A(p') \quad \forall A \quad (1)$$

continues to hold under the time evolution of the process, we call the family of processes monotone with respect to the parameter $p$. If a family of processes is monotone with respect to some parameter $p$, we can use the technique described above to simulate them for all values of $p$ (in a given range) at the same time!

Obviously, not all interacting stochastic processes are monotone with respect to a suitable parameter—indeed, monotonicity with respect to a parameter necessarily implies that the process itself must be monotone with respect to its initial condition (Liggett, 1999), which many stochastic processes are not. (For example, processes that exhibit cyclic dynamics are generally not monotone.) However, the basic contact process is indeed monotone, both in itself and with respect to several parameters of interest, such as the contact rate $c$ and the recovery rate $r$, as well as any parameter $p$ such that $c$ is an increasing and $r$ a decreasing function of $p$ (or vice versa).

![Figure 3](image)

**Figure 3:** Examples of possible local transition events in a monotone coupled contact process simulation with $r$ as the coupling parameter. The bars represent the state of a site, with the shaded area showing the parameter range for which that site is infected. On each recovery event, a threshold value $r_{crit}$ is chosen uniformly between 0 and $r_{max}$ and the focal site is marked as uninfected for all $r \geq r_{crit}$.

**Algorithm 3:** Monotone coupling simulation for the contact process with $0 \leq r \leq r_{max}$, fixed $c$.

```plaintext
Data: $\theta_x \in [0,r_{max}] \quad \forall x \in L = \{1, \ldots, N\}$
while $t < t_{max}$ do
    $A :=$ random site in $L$
    $x :=$ random number in $[0,r_{max} + c]$
    if $x < c$ then
        $A$ unconditionally infects $B$:
        $B :=$ random neighbor of $A$
        $\theta_B \leftarrow \max(\theta_A, \theta_B)$
    else
        $A$ recovers if $r \geq r_{crit} = x - c$:
        $\theta_A \leftarrow \min(\theta_A, x - c)$
    end
    $t \leftarrow t + \frac{1}{(r_{max} + c)N}$
end
```

As an example, algorithm 3 shows how to simulate the basic contact process for all values of $r \in [0,r_{max}]$ for a fixed $c$. Here, the state vector $S_A$ from algorithm 2 is replaced by the threshold value $\theta_A$, which stores the smallest value of the coupling parameter $r$ for which the site $A$ is not currently occupied.

Figure 3 shows the types of events that occur in this simulation. On contact events, the threshold value $\theta_B$ of the target site $B$ is simply raised up to the threshold $\theta_A$ of the infecting site $A$, showing...
that \( B \) is now infected in (at least) all the coupled processes in which \( A \) was infected before the event. On recovery events, we reduce the threshold value \( \theta_A \) down to a random value \( r_{\text{crit}} \) uniformly chosen between 0 and \( r_{\text{max}} \). Conveniently, we already have such a random variable available: the variable \( x \) is uniformly distributed between \( c \) and \( r_{\text{max}} + c \), so we can simply let \( r_{\text{crit}} = x - c \). In this way, only the fraction \( r/r_{\text{max}} \) of all recovery events affect the state of the process with parameter \( r \). Since the total rate of recovery events in algorithm 3 is \( r_{\text{max}} \) per site, the effective per site recovery rate for the process with parameter \( r \) is indeed \( r \).

**Algorithm 4:** Monotone coupling simulation for the contact process with \( 0 \leq c \leq c_{\text{max}} \), fixed \( r \).

**Data:** \( \theta_x \in [0, c_{\text{max}}] \quad \forall x \in L = \{1, \ldots, N\} \)

while \( t < t_{\text{max}} \)

\( A := \) random site in \( L \)

\( x := \) random number in \([0, r + c_{\text{max}}]\)

if \( x < c_{\text{max}} \) then

\( A \) infects \( B \) if \( c < c_{\text{crit}} = x \):

\( B := \) random neighbor of \( A \)

\( \theta_B \leftarrow \min(\theta_B, \max(x, \theta_A)) \)

else

\( A \) recovers unconditionally:

\( \theta_A \leftarrow c_{\text{max}} \)

end

\( t \leftarrow t + \frac{1}{(r + c_{\text{max}})N} \)

end

Algorithm 4 simulates the same process for \( c \in [0, c_{\text{max}}] \) and fixed \( r \). Here \( \theta_A \) denotes the smallest value of \( c \) for which the site \( A \) is occupied; \( \theta_A = c_{\text{max}} \) means that the site \( A \) is not currently occupied in any of the coupled processes. Figure 4 illustrates the events possible in this algorithm: recovery events occur independently of the coupling parameter \( c \), while on contact events, we choose a uniform random value \( c_{\text{crit}} \) between 0 and \( c_{\text{max}} \) (for which purpose, again, the uniform random variable \( x \) is already conveniently available) and lower the infection threshold \( \theta_B \) of the target site \( B \) down to the maximum of \( c_{\text{crit}} \) and the infection threshold \( \theta_A \) of the focal site \( A \). Thus, a fraction \( c/c_{\text{crit}} \) of all contact events affect a process with the coupling parameter value \( c \), giving that process the effective contact rate \( c \).

4. Multitype contact processes

The monotone coupling technique is not restricted to the basic single-type contact process. The challenge in applying it to more complicated processes is mainly in finding a suitable parameter which changes the dynamics in a nontrivial, yet monotone, manner. Fortunately, many processes do have such a parameter, even if it may not always be the most interesting one. If the goal is to explore the entire parameter space, the existence of any monotone parameter—even if trivial—allows much more efficient sampling of the parameter space than if no such parameters exist.

For processes featuring two competing (and mutually exclusive) infectious strains \( a \) and \( b \), with the respective infection and recovery rates \( c_a, r_a \) and \( c_b, r_b \), a sufficient condition for the process to be monotone with respect to a parameter \( p \) is that \( c_a \) and \( r_b \) are (weakly) decreasing and \( r_a \) and \( c_b \) (weakly) increasing functions of \( p \). If this condition holds, we may order the possible states of a single lattice site as follows:

1. infected with strain \( a \),
2. not infected,
3. infected with strain \( b \),

and arrange all transitions of the coupled process to preserve the monotonicity property (1).

Quite a few well known models possess such parameters. For example, the infection rates \( \lambda_1 \) and \( \lambda_2 \) in the original multitype contact process defined
by Neuhauser (1992) are both monotone parameters. So is the cost of altruism \( C \) in the model of van Baalen and Rand (1998).

In some cases, the same technique can be applied to processes with more than two competing strains. For example, in the three-strain model of Lanchier and Neuhauser (2006) for generalist–specialist coexistence on two site types, the two specialist strains are each restricted to their respective site types, and can thus be effectively treated as a single strain that cannot spread from one site type to another. In Karonen (2012) I have applied the monotone coupling technique to simulating a process essentially equivalent to that of Lanchier and Neuhauser (2006), with the generalist infection probability \( p \in [0, 1] \) as the coupling parameter.

Algorithm 5 shows a simplified version of the algorithm used to simulate the process studied in Karonen (2012). (The original implementation also uses occupancy / vacancy lists and various other optimizations.) In this model, the sites are arbitrarily divided into two classes, and the strains consists of two specialists, only capable of infecting sites of the corresponding class, and a generalist strain capable of infecting either class of sites with equal (but reduced compared to the specialists) probability. No superinfection is assumed to occur. Thus, each site can be considered to be in one of three states: infected by a specialist strain (1), uninfected (2), or infected by the generalist strain (3). (Each class of sites can only be infected by one of the specialist strains, so it is not necessary to track which specialist has infected a given site.) With the site states numbered as above, this process is monotone with respect to the infection probability \( p \in [0, 1] \) of the generalist strain.

Here, \( H_A \in \{0, 1\} \) is the type of the site \( A \) (which does not change during the simulation), and \( \theta_A = (\theta_A, \theta_A) \) denotes the threshold values of the coupling parameter \( p \) at which the current state of the site \( A \) changes: for \( p < \theta_A \) the site is infected by a specialist, for \( p \geq \theta_A \) it is infected by the generalist, and for intermediate values of \( p \) it is uninfected.

The function \( \text{med}(x, y, z) \) returns the median of its inputs, and is in effect used to "clamp" \( y \) to the interval \([x, z]\), so that, if \( y \) lies outside the interval, the closest endpoint is taken instead. This is done so that, if the effective infection threshold lies outside the uninfected range \([\theta_B, \theta_B]\) of the target site \( B \), either no infection takes place or the infection happens for the entire range, as shown in Figure 5. In particular, this ensures that \( \theta_{A, 1} \leq \theta_{A, 2} \) stays true for all sites \( A \), provided that the initial state satisfies this.

5. Efficient statistics collection

The purpose of simulating a stochastic process is to collect some data about it. In some cases, the data we wish to collect, such as the presence or absence of a certain strain, can be obtained simply from the final state of the process after simulating it for \( t_{\max} \) time units. More commonly, however, we wish to average some quantities, such as population densities, over a period of time, if only to reduce the effects of stochastic fluctuations.

Of course, one way to accomplish this is to simply run the process for some time interval \( \delta t \), sample the values of interest from the lattice state at that point, and repeat until enough samples have been collected. However, while easy to implement, this method is somewhat inefficient. If \( \delta t \) is small, successive samples will be highly correlated, and so we will need to collect many of them to average out temporal fluctuations. Since each sampling step usually involves iterating over the entire lattice, this can consume a lot of time if done frequently. On the

\[ A := \text{random site in } L \]
\[ x := \text{random number in } [0, r + c) \]
\[ \begin{cases} B := \text{random neighbor of } A & \text{if } H_A = H_B \text{ then} \\ & \text{specialist always infects if host types match:} \\ & \theta_{B, 1} \leftarrow \text{med}(\theta_{B, 1}, \theta_{A, 1}, \theta_{B, 2}) \\ & \theta_{B, 2} \leftarrow \text{med}(\theta_{B, 1}, \max(x/c, \theta_{A, 2}), \theta_{B, 2}) \end{cases} \]
\[ \text{else} \]
\[ A \text{ recovers unconditionally:} \]
\[ \theta_{A, 1} \leftarrow 0, \theta_{A, 2} \leftarrow 1 \]
\[ t \leftarrow t + \frac{1}{N(r+c)} \]

| Algorithm 5: Monotone coupled simulation for a multitype contact process with generalist infectivity \( 0 \leq p \leq 1 \), fixed \( c \) and \( r \) |
|---|
| **Data:** \( \theta_{x} \in [0, 1]^2 \forall x \in L = \{1, \ldots, N\} \) |
| **while** \( t < t_{\max} \) **do** |
| \( A := \text{random site in } L \) |
| \( x := \text{random number in } [0, r + c) \) |
| **if** \( x < c \) **then** |
| \( B := \text{random neighbor of } A \) |
| **if** \( H_{A} = H_{B} \) **then** |
| specialist always infects if host types match: |
| \( \theta_{B, 1} \leftarrow \text{med}(\theta_{B, 1}, \theta_{A, 1}, \theta_{B, 2}) \) |
| \( \theta_{B, 2} \leftarrow \text{med}(\theta_{B, 1}, \max(x/c, \theta_{A, 2}), \theta_{B, 2}) \) |
| **else** |
| \( A \text{ recovers unconditionally:} \) |
| \( \theta_{A, 1} \leftarrow 0, \theta_{A, 2} \leftarrow 1 \) |
| **end** |
| **end** |

6
Somewhere between these two extremes there presumably exists an optimal value of $\delta$, which also consumes time. On the other hand, if $\delta$ is large, we need to simulate the process longer to collect a given number of samples, which also consumes time.

Somewhere between these two extremes there presumably exists an optimal value of $\delta$ (for a particular process) that minimizes the amount of computation needed to achieve a given noise level. However, rather than optimizing $\delta$, what we’d really like to do would be to calculate the true average of the values we’re interested in over a given time interval while simulating the process.

One way to do this is to observe that every infected site is sampled (at least) twice during the course of each infection: once when the infection occurs, and once when the site recovers. If the mean infection length $\bar{\tau} = 1/r$ is known and significantly shorter than the timespan $t$ which we are averaging over, simply counting the number $n$ of successful infection (or recovery) events during the interval and multiplying it with $\bar{\tau}/Nt$ (where $N$ is the number of sites in the lattice) will yield a very good estimate of the average infection density over the chosen time interval.

Such counting can be easily incorporated into the naïve algorithm 1 simply by incrementing a (realization and strain specific) counter whenever the state of a site changes (in the direction we are counting). However, applying it to the monotone coupled simulation algorithms in section 3 and section 4 is slightly less trivial, since we are simulating many (conceptually infinitely many) realizations of the process at the same time: obviously, storing a counter for each of them and incrementing all those for which a change occurs would be inefficient.

Instead, we can make use of the observation that, whenever a site state change occurs in the coupled simulation algorithms, it is always over a contiguous range of values of the coupling parameter (or possibly a small number of disjoint ranges, as in algorithm 5). Thus, to record the parameter range for which an event occurs, it suffices to increment a counter corresponding to the start of the range and to decrement the counter corresponding to its end. We can then obtain the number of events that have occurred for a given parameter value simply by summing up the counters corresponding to parameter values below it.

Algorithm 6 shows a variant of algorithm 4 with this event counting implemented for both infection and recovery events. The parameter range $[0, \theta_{\text{max}}]$ is divided into segments of length $\delta$, with the array $n_1, \ldots, n_{\theta_{\text{max}}/\delta}$ of counters counting infection events while the array $m_1, \ldots, m_{\theta_{\text{max}}/\delta}$ counts recovery events. (Of course, in practice one would only track one of these event types, since the difference between the event counts can be more easily obtained simply by counting the number of infected sites before and after the time interval of interest.) At the end of the simulation, $\sum_{i=1}^{k} n_i$ gives the number of infection events, and $\sum_{i=1}^{k} m_i$ the corresponding number of recovery events, that have occurred for the parameter value $c = k\delta$.

Of interest is the fact that, as recovery events in algorithm 4 are always unconditional, we need not record the endpoint of the affected range, since it is always $\theta_{\text{max}}$. This saves time, and makes track-
Algorithm 6: Variant of algorithm 4 (monotone coupling simulation for the contact process with $0 < c < c_{\text{max}}$, fixed $r$) with event counting.

Data: $\theta_x \in [0, c_{\text{max}}]$ \quad $\forall x \in L = \{1, \ldots, N\}$

$n_i \in \mathbb{Z}$ \quad $\forall i \in \{1, \ldots, \lceil c_{\text{max}}/\delta_i \rceil \}$

$m_i \in \mathbb{Z}$ \quad $\forall i \in \{1, \ldots, \lceil c_{\text{max}}/\delta_c \rceil \}$

while $t < t_{\text{max}}$ do

$A :=$ random site in $L$

$x :=$ random number in $[0, r + c_{\text{max}})$

if $x < c_{\text{max}}$ then

$A$ infects $B$ if $c < c_{\text{crit}} = x$:

$B :=$ random neighbor of $A$

$\theta_{\text{new}} := \max(x, \theta_A)$

if $\theta_B > \theta_{\text{new}}$ then

$n[\theta_{\text{new}}/\delta_i] \leftarrow n[\theta_{\text{new}}/\delta_i] + 1$

$n[\theta_B/\delta_i] \leftarrow n[\theta_B/\delta_i] - 1$

$\theta_B \leftarrow \theta_{\text{new}}$

end

else

$A$ recovers unconditionally:

$m[\theta_A/\delta_i] \leftarrow m[\theta_A/\delta_i] + 1$ if $\theta_A < c_{\text{max}}$

$\theta_A \leftarrow c_{\text{max}}$

end

$t \leftarrow t + \frac{1}{(r + c_{\text{max}})N}$

end

6. Discussion

Even though the basic principle of simulating interacting stochastic processes on a computer is simple and straightforward, doing it efficiently can be surprisingly complicated. The coupled simulation technique described here, and in particular the monotone coupling technique described in section 3 and section 4, are useful tools that can substantially speed up the simulation of certain common types of contact processes by allowing the simulation of many parametrized variants of the process at the same time.

There is no single algorithm that would be optimal for simulating all possible interacting stochastic processes (or, at least, the author is not aware of any such thing). The usefulness and applicability of the techniques described in this paper will have to be individually evaluated for each particular class of processes one is interested in simulating.

This paper does not attempt to provide a comprehensive description of all the optimization techniques available for simulating interacting stochastic processes. There are several well known optimization techniques, such as the occupancy lists briefly mentioned in section 1, which are more or less orthogonal to the techniques presented in this paper and can (and should) be combined with them where applicable.

While I have mainly used the classical lattice contact process of Harris (1974) as the canonical example with which to demonstrate these simulation techniques, section 4 demonstrates that, even though the monotone coupling technique in particular requires certain rather specific properties of the process, they are nonetheless applicable to a wider range of ecological models.

Although this paper is written mainly with discrete lattice models in mind, there seems to be no reason why the techniques described here could not be naturally adapted to simulations of spatio-temporal point processes in continuous space (Dieckmann et al., 1997). Indeed, such processes can be viewed as a limiting case of lattice models as the number of sites per area tends to infinity. Of course, with infinitely many sites, sampling from the entire set of sites will not be feasible, so that the use of an occupancy list, which was mentioned as an optimization technique in section 1, becomes a necessary part of the simulation algorithm. Also, to implement density regulation, the handling of contact events must be modified to account for the suppression of offspring growth in areas close to existing individuals. Still, these are both standard features of any spatio-temporal point process simulation algorithm, and should not interfere with the coupling technique in any way.

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