Markov-chain Monte Carlo is one of the most widely used computational methods in the natural sciences. It samples a high-dimensional space of configurations $c$ according to a probability distribution $\pi(c)$. In the physical sciences, $\pi$ generally corresponds to the Boltzmann distribution $\pi(c) = \exp[-\beta E(c)]$, where $\beta$ is the inverse temperature and $E$ the system energy. The core of most Monte Carlo computations is the Metropolis algorithm $\dagger$, which accepts a trial move from configuration $i$ to configuration $f$ with probability

$$p^{\text{Met}}(i \to f) = \min\{1, \exp[-\beta(E(f) - E(i))]\}. \tag{1}$$

The acceptance probability Eq. 1 satisfies the detailed balance condition, $\pi(i)p^{\text{Met}}(i \to f) = \pi(f)p^{\text{Met}}(f \to i)$, that leads to exponential convergence towards the stationary distribution $\pi(c)$, if ergodicity is assured $\ddagger$. Moving from one configuration to another requires evaluating the induced change of the system energy. In most classical $N$-particle simulations, the system energy is a sum over pair terms: $E = \sum_{(k,l)} U_{kl} = \sum_{(k,l)} U(r_{kl})$ with the pair potential $U$ and the interparticle distances $r_{kl} = r_i - r_k$. The evaluation of the system energy generally takes $O(N^2)$ operations, and the computation of the energy change upon moving a single particle takes $O(N)$ operations. For a potential with finite support, the change of the system energy for moving one particle is computed in $O(1)$. To speed up the evaluation, potentials with infinite support, such as the Lennard-Jones and other moderately long-ranged potentials, are truncated beyond an effective interaction range. This approximation is however known to alter the equilibrium properties $\ddagger\ddagger$. Strongly long-ranged potentials, as they appear in electrostatics and gravity, do not allow for the definition of a finite interaction range and require specialized techniques for determining the system energy to high precision. Ewald summation $\ddagger\ddagger\ddagger$, for example, adds and subtracts smooth charge distributions localized around the point particles. With periodic boundary conditions, this turns the long-ranged part of the interaction into a rapidly converging sum in Fourier space. Ewald summation computes the system energy in $O(N^{3/2})$, taking into account periodically replicated images of the particles $\ddagger\ddagger\ddagger\ddagger$. Its refinements further reduce the burden of the system-energy computation by discretizing the charge density $\ddagger\ddagger\ddagger\ddagger$ or by exploiting large-scale uniformity $\ddagger\ddagger\ddagger\ddagger$. Still, in many outstanding applications in the natural sciences, the evaluation of long-ranged potentials remains a computational bottleneck. Implementing Ewald summation is particularly difficult if periodic boundary conditions are not realized in all dimensions, as for example in slab geometries $\ddagger\ddagger\ddagger\ddagger\ddagger$.

In this paper, we present a rigorous Monte Carlo algorithm for $NVT$ particle systems with long-ranged interactions that does not evaluate the system energy, in contrast to virtually all existing Markov-chain Monte Carlo algorithms $\ddagger\ddagger\ddagger\ddagger\ddagger$. This change of perspective opens up many opportunities: Based on a cell-veto scheme within the factorized Metropolis algorithm $\ddagger\ddagger\ddagger\ddagger\ddagger$, it implements a single-particle move in complexity $O(1)$ without any truncation error. For moderately long-ranged potentials, such as Lennard-Jones or dipolar interactions, the step size is independent of the system size, and the algorithm is effectively constant-time. For strongly long-ranged interactions, as the Coulomb forces, the single-move step size slightly decreases with $N$. For concreteness, we will consider a fixed hypercubic box of size $L^D$ with periodic boundary conditions, where $D$ is the dimension of physical space. The generalization to slab geometries is straightforward.

In contrast to the Metropolis algorithm of Eq. 1 the pairwise factorized algorithm $\ddagger\ddagger\ddagger\ddagger\ddagger$ accepts moves with the probability

$$p^{\text{fact}}(i \to f) = \prod_{(k,l)} \min\{1, \exp[-\beta \Delta U_{kl}(i \to f)]\}, \tag{2}$$

where $\Delta U_{kl}$ is the change in the pair potential between particles $k$ and $l$. In our algorithm, we never explicitly evaluate the function $p^{\text{fact}}$. Rather, the product of probabilities on the rhs of Eq. 2 is interpreted as a condition that is true if all its factors are true. The move $i \to f$ is thus accepted by consensus, namely if each pair $(k,l)$

\textbf{Cell-veto Monte Carlo algorithm for long-range systems}

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We present a rigorous efficient event-chain Monte Carlo algorithm for long-range-interacting particle systems. Using a cell-veto scheme within the factorized Metropolis algorithm, we compute each single-particle move with a fixed number of operations. For slowly decaying potentials such as Coulomb interactions, screening line charges allow us to take into account periodic boundary conditions. We discuss the performance of the cell-veto Monte Carlo algorithm for general inverse-power-law potentials, and illustrate how it provides a new outlook on one of the prominent bottlenecks in large-scale atomistic Monte Carlo simulations.
independently accepts the move with probability $p_{kl}$ [12] (see Fig. 1). Instead of computing the energy to high precision, we will compute upper bounds for the veto probability $1 - p_{kl}$ by embedding particles $k$ and $l$ into cells $C_k$ and $C_l$, respectively. To identify particles vetoing the move, one rapidly identifies cell vetos and inspects the contents of corresponding cells to determine whether the cell vetos are confirmed on the particle level (see Fig. 1).

In continuum space, two configurations $i$ and $f$ with $i \neq f$ can be infinitesimally close to each other. For regular potentials, this implies that the change of pair energies $\Delta U_{kl}(i \rightarrow f)$, and therefore the veto probability $1 - p_{kl}$, are infinitesimal as well. In the event-chain algorithm [12, 13], a proposed move $i \rightarrow f$ consists in the infinitesimal displacement of an “active” particle $a$ in a direction $\hat{e}$: The proposed move is $r_a(i) \rightarrow r_a(f) = r_a(i) + \hat{e} \Delta s$, where $\Delta s$ is an infinitesimal time increment. The active particle keeps moving in the same direction until a move is finally vetoed by a target particle $t$. The target particle then becomes the new active particle, i.e., the proposed move is $(i, a, \hat{e}) \rightarrow (f, a, \hat{e})$, and if vetoed by particle pair $(a, t)$, the configuration is changed to $(i, t, \hat{e})$. This implements a “lifted” Markov chain [14] with two additional variables $a$ and $\hat{e}$, which trivially projects to the physical space with the proper Boltzmann distribution. Veto probabilities $1 - p_{at}$ are infinitesimal.

Two simultaneous vetos are thus prevented from arising from different target particles. Detailed balance is violated (the reverse move $r_a(f) = r_a(i) - \hat{e} \Delta s$ is never proposed). However, the event-chain algorithm satisfies the global-balance condition

$$\sum_i \pi(i)p(i \rightarrow f) = \pi(f)$$

sufficient for exponential convergence to the equilibrium distribution on the accessible configurations. To ensure ergodicity, both the active particle and the direction of motion are periodically reset to random values (see Supp. 2). Lifted Markov chains have been shown to improve convergence speed in many cases, and also to lower the dynamical critical scaling exponents [14–17].

The core of an event-chain program consists in determining the step size $\Delta s$ to the next particle event and in identifying the vetoing target particle $t$, rather than explicitly programming small time increments (see Fig. 2). The actual move then merely consists in updating the active particle position as $r_a \rightarrow r_a + \hat{e} \Delta s$ and in changing the active particle to $t$. For long-ranged potentials, $\Delta s$ can be far away from the active particle. At any instant during the simulation, the veto probability of a potential target particle $t$ is given by the particle-event rate $q$, defined via a directional derivative of the pair potential,

$$1 - p_{at} = q(r_{at}) \Delta s = \beta [ -\hat{e} \cdot \nabla U_{at}]^+ \Delta s$$

with $[\cdot]^+ = \max(0, \cdot)$. For long-ranged potentials, $q$ carries over large distances (see Fig. 2b, c). Particle-event distances $r_{at}$ are distributed as $q(r_{at})g(r_{at})$, where $g$ is the radial distribution function, and thus exhibit the same long-ranged tail. In contrast, the displacement between events, i.e., the step size $\Delta s$, decays exponentially within a few interparticle distances, see Fig. 2. For each pair $(a, t)$, the event time $\Delta s$ can be computed in $O(1)$, so that the event-chain algorithm can be implemented in $O(N)$ per particle event [18], by iterating over all target particles. The earliest veto will define the step size $\Delta s$ and the active particle for the next step.

For a homogeneous system (with a bounded particle density), the complexity per particle event can be re-
duced from \( \mathcal{O}(N) \) to \( \mathcal{O}(1) \) by establishing upper bounds for the particle-event rate which hold irrespective of the precise particle positions. Concretely, we superimpose a fixed regular grid onto the system, with cells typically containing at most one particle (see Fig. [1] rare “surplus” particles are treated separately). The particle-event rate between the active particle in cell \( C_a \) and a target particle in cell \( C_t \) is bounded from above by the cell-veto rate

\[
Q(C_a, C_t) = \max_{r_a \in C_a, r_t \in C_t} q(r_t - r_a). \tag{5}
\]

This quantity depends only on the pair potential and the relative positions of the two cells and can be tabulated before sampling starts. The cell-veto rate remains finite except for a few nearby cells that contain the hard-core singularities. In the case of point particles, these must include any cells that share corners with \( C_a \) (see Fig. [1]). For efficiency, “nearby” cells may comprise a larger portion of the short-range features of \( U \).

Excluding nearby and surplus particles, the total particle-event rate is bounded from above by the total cell-veto rate

\[
Q_{\text{tot}} = \sum_{C_t} Q(C_a, C_t), \tag{6}
\]

which remains a constant throughout the simulation. The next cell veto can then be sampled in \( \mathcal{O}(1) \): The time is distributed exponentially

\[
P(\Delta s) = Q_{\text{tot}} \exp (-Q_{\text{tot}} \Delta s), \tag{7}
\]

so that \( \Delta s \) is given through the logarithm of a uniform random number (2, see Supp. 2). The cell veto is triggered by the cell \( C_t \) with probability \( \sim Q(C_a, C_t) \). The selection of the target cell from all the non-nearby cells can also be accomplished in constant time (see below). If the vetoing cell \( C_t \) contains a particle, at position \( r_t \), it is then chosen as the target particle for a particle event with probability \( q(r_a + \hat{e} \Delta s, r_t)/Q(C_a, C_t) \). This long-range particle event must be put into competition with events triggered by nearby or surplus particles, which are handled as in the short-range event-chain algorithm (see also Supp. 2). The number of nearby particles is naturally bounded. The number of surplus particles may remain constant throughout the simulation. Consequently, a cell veto can effectively be processed constant time, and the performance of the cell-veto algorithm depends on the rate of cell vetos \( Q_{\text{tot}} \).

The total cell-veto rate \( Q_{\text{tot}} \) depends on the range of the pair potential. For inverse-power-law interactions, \( U(r) \sim 1/r^n \), the event rate for a bare particle scales as \( q \sim 1/r^{n+1} \) \([19]\). In an infinite system, the total cell-veto rate \( Q_{\text{tot}} \sim \int d^n r q \) is finite for moderately long-ranged potentials, i.e., for \( n > D - 1 \). This class includes dipolar forces in \( D = 2 \) and \( D = 3 \), as well as the Lennard-Jones potential. In this case, the cell-veto algorithm is of complexity \( \mathcal{O}(1) \).

![Figure 3](image-url) (Color online) a) Total cell-veto rate \( Q_{\text{tot}} \), Eq. (5) for inverse-power-law potentials in \( D = 2 \). The event rate for bare particles diverges as \( n \to D - 1 \) (vertical line) because of the presence of periodic images, while screened event rates stay finite. Solid bullets are the Coulomb system \( (n = D - 2) \); for \( 2D \), \( U(r) \sim -\ln r \). b) Scaling of \( Q_{\text{tot}} \) with system size \( N \), for the screened-lattice algorithm (green solid), and for the bare-particle algorithm (purple dashed). The inclined line is \( \sim N^{1/2} \).

For strongly long-ranged potentials \( n \leq D - 1 \), including Coulomb forces), the cell-veto rate in an infinite system diverges (see Fig. [3]). In the replicated-box representation of periodic boundary conditions (see Fig. [1]), even the sum over all periodic images of a single target particle \( (N = 2) \) leads to an infinite particle-event rate. The sum may be regularized by adding uniformly charged line segments (parallel to the direction of motion \( \hat{e} \)) that neutralize each particle charge yet combined leave invariant the energy differences of the original system. Screening line charges can be defined for general potentials. For inverse-power-law interactions, the directional derivatives of the particle and line-charge potentials are

\[
\langle \hat{q}(r) \rangle = \beta d^n \times \frac{\hat{e} \cdot r}{r^{n+2}}, \tag{8}
\]

\[
\langle \bar{l}(r) \rangle = \frac{\beta}{L} \times \left[ U(r + \hat{e}L/2) - U(r - \hat{e}L/2) \right], \tag{9}
\]

where \( r \) is the folded-out distance vector between the active particle and a particular periodic image of the target particle. By vanishing monopole and dipole moments, \( \hat{q} + \bar{l} \) asymptotically decays as \( 1/r^{n+3} \), sufficient to render \( Q_{\text{tot}} \) unconditionally convergent for Coulomb forces.

We may now define three distinct particle-event rates:

\[
q(r) = \begin{cases} 
\langle \hat{q}(r) \rangle^+ & \text{bare,} \\
\langle \hat{q}(r) \rangle^+ + \langle \bar{l}(r) \rangle^+ & \text{screened,} \\
\sum_k \langle \hat{q}(r_k) \rangle^+ & \text{screened lattice. (10)}
\end{cases}
\]

The screened-lattice version of Eq. (8), where the sum extends over all periodic images of the target particle,
minimizes the cell-veto rate by merging the periodic images into the primary copy of each particle. The number of target cells $C_t$ is finite, and the target cell of a cell veto can be found extremely efficiently by precomputing the function $Q(C_a, C_t)$ and employing Walker’s alias method or related techniques \[20\, 21\] (see Supp. 1). A commented Python implementation of the cell-veto Monte Carlo algorithm using this approach is provided in Supp. 2.

In an alternative version of the cell-veto algorithm, the particle-event rates of Eq. \[10\] and Eq. \[11\] are used with explicitly replicated simulation boxes. An infinite number of target cells is considered. The target cell for a cell veto can be handled in $O(N)$ event rates overcome the divergence at $n = D - 1$ energy. Remarkably, it advances the physical state of the system by one event in $O(1)$ even for long-ranged interactions. The algorithm introduces none of the cut-offs that come with practical versions of Ewald summation. Strongly long-ranged potentials such as electrostatic forces are handled exactly using screening line charges. The complexity of the algorithm then scales weakly with $N$. It is hoped that the algorithm will permit to access much larger systems than was previously possible. The demo program of Supp. 2, and the C++ version of this algorithm are available online \[22\].

In conclusion, we have presented a cell-veto Monte Carlo algorithm that need not compute the system energy.

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\[22\] https://github.com/Cell-veto.
Supplementary Item 1: Cell-veto sampling

The pairwise factorized Metropolis algorithm determines pair events (vetos) and thus avoids to compute the system energy. The cell-veto algorithm takes this strategy one step farther. Instead of scanning all particle pairs for vetos, it first solicits cell vetos (see Fig. 1), which then have to be confirmed on the level of the actual particle positions. Even with periodic boundary conditions, the number of cells remains finite if all the periodic images of a particle are merged into the one located in the primary simulation box (see Eq. (12)). The next cell veto must be selected from the $N_{\text{cell}}$ cells $C_t$ with a nonzero cell-veto rate. Each cell must be sampled with probability $\sim Q(C_a, C_t)$, see Fig. [S1]. This finite discrete-probability sampling problem is best solved through a rejection-free exact algorithm, as Walker’s alias method. In Walker’s method, the cell-veto rates are reassembled into composite rates consisting of at most two original rates and adding up to exactly the mean cell-veto rate $Q_{\text{mean}} = Q_{\text{tot}} / N_{\text{cell}}$. The cutting-up and reassembling of the $Q(C_a, C_t)$ constitutes the initialization stage of Walker’s method (in the demo program of Supp. 2: in function `WalkerSet`). In the sampling stage, a cell $C_t$ can be sampled with the proper probability by first sampling the composite rate (as a random integer between 1 and $N_{\text{cell}}$) and then deciding between the at most two rates by sampling a uniform random real between 0 and $Q_{\text{mean}}$ (WalkerSample, in the demo program of Supp. 2). This step is constant time and independent of the number of cells.

FIG. S1. Cell-veto sampling using Walker’s method. Left: The non-nearby cells (5 such cells shown in different colors) may all have finite cell-veto rates. Center: Cell-veto rates in a linear representation. The mean cell rate $Q_{\text{mean}}$ is indicated (5 cells shown, again). Right: In the initialization stage of Walker’s method, the cell rates are reassembled, at most by pairs, into composite rates.

FIG. S2. Cell-veto sampling using rejection sampling with a function $Q(x)$ in a “folded-out” periodic system and an infinite number of cells (one-dimensional representation shown).
Alternatively, one may also keep the individual cells, that is, work explicitly in the folded-out version of the system, and with the cell-veto rates of Eq. (11) that consider each periodic copy of a target cell individually. The number of cells is now countably infinite. Nevertheless, it is easy to devise a rejection-sampling strategy using a function that is easy to sample, integrable to infinity, and an upper bound to the cell-veto rate (see Fig. S2 for a one-dimensional representation). A point $x$ sampled from the probability distribution $\sim Q(x)$ identifies a cell. If that cell contains a target particle $t$, a particle event is triggered with probability $q(r_t) / V_{\text{cell}} / Q(x)$. In the folded-out formulation of the cell-veto algorithm, surplus particles must still be merged with their periodic images, in order to keep their number finite.

Supplementary Item 2: Demo implementation of the cell-veto algorithm

The demo implementation of the cell-veto Monte Carlo algorithm, the program `demo_cell.py`, is written in the Python 2 programming language. $N$ particles are simulated in a two-dimensional square box of length 1 with periodic boundary conditions, and with an $1/r$ pair potential that is periodically continued. A regular square grid with $L^2$ cells is superimposed to the system. Cells are numbered from 0 to $L^2 - 1$. The screened-lattice particle-event rate of Eq. (12) is implemented (naively). Walker’s method is used for sampling the veto cells.

In the setup stage of `demo_cell.py`, particles are initialized to random positions, and the cell-veto rates are computed between the active cell $C_a = 0$ and all other target cells that are not nearby $C_a = 0$. The function `translated_cell` transfers this calculation (with $C_a = 0$) to arbitrary cell pairs $(C_a, C_t)$. Specifically, the cell-veto rate is defined as the maximum of the particle-event rate over all positions, as indicated in Eq. (5). For this demo program, it is assumed that the maximum particle-event rate is attained for $x_a$ and $x_t$ on the boundary of $C_a$ and $C_t$, respectively, and discrete points in the list `cell_boundary` are used. For the demo version, the lattice-screened particle-event rate of Eq. (12) is determined by a naive direct summation of the images of the target particle and its screening line charge (see function `pair_event_rate`), rather than by an efficient function evaluation. The initialization of Walker’s alias method, as explained in Supp. 1, concludes the setup stage of `demo_cell.py`.

In one iteration of the sampling stage of `demo_cell.py`, particles advance by a total distance `chain_ell` (see [12, 13]) in a fixed direction. This direction of motion is first sampled (from $+x$ or $+y$). In the demo version, only the $+x$ move is implemented explicitly ($+y$ moves are implemented indirectly by flipping all particle coordinates $(x_i, y_i) \rightarrow (y_i, x_i)$). At the beginning of this iteration (given that such a flip may have taken place) particles are reclassified into target particles associated to cells (at most one per cell), and surplus particles. (Each cell must contain at most one particle, in order for the cell-veto rate to be an upper limit for the particle-event rate from all particles within the cell). The active particle is then sampled uniformly among all particles in the system. At each step of the iteration, the step size `delta_s` to the next cell veto is sampled from the total cell-veto rate $Q_{\text{tot}}$. The cell veto may be preempted by the end of the chain, after displacement `chain_ell`. It is also checked whether the cell veto occurs after the active particle crosses the cell limit: We must trigger an event when the cell boundary is reached, as the set of nearby particles then changes. If the cell veto is indeed confirmed on the particle level, it is put into competition with events triggered by nearby or surplus particles. In the demo version, the particle-event rates for nearby or surplus particles are computed in a simplified way.

The `demo_cell.py` program (see below) was tested against a straightforward implementation of the Metropolis algorithm, and against the C++ version (see https://www.github.com/cell-veto/postlhc/).

```python
import math, random, sys
import numpy as np

def norm (x, y):
    """norm of a two-dimensional vector""
    return (x*x + y*y) ** 0.5

def dist (a, b):
    """periodic distance between two two-dimensional points a and b""
    delta_x = (a[0] - b[0] + 2.5)% 1.0 - 0.5
    delta_y = (a[1] - b[1] + 2.5)% 1.0 - 0.5
    return norm (delta_x, delta_y)

def random_exponential (rate):
```
return -math.log(random.uniform(0.0, 1.0)) / rate

def pair_event_rate(delta_x, delta_y):
    """compute the particle event rate for the 1/r potential in 2D (lattice-screened version)""
    q = 0.0
    for ky in range(-k_max, k_max + 1):
        for kx in range(-k_max, k_max + 1):
            q += (delta_x + kx) / norm(delta_x + kx, delta_y + ky) ** 3
            q += 1.0 / norm(delta_x + kx + 0.5, delta_y + ky)
            q -= 1.0 / norm(delta_x - kx - 0.5, delta_y + ky)
    return max(0.0, q)

def translated_cell(target_cell, active_cell):
    """translate target_cell with respect to active_cell""
    kt_y = target_cell // L
    kt_x = target_cell % L
    ka_y = active_cell // L
    ka_x = active_cell % L
    del_x = (kt_x + ka_x) % L
    del_y = (kt_y + ka_y) % L
    return del_x + L*del_y

def cell_containing(a):
    """return the index of the cell which contains the point a""
    k_x = int(a[0] * L)
    k_y = int(a[1] * L)
    return k_x + L*k_y

def walker_setup(pi):
    """compute the lookup table for Walker’s algorithm""
    N_walker = len(pi)
    walker_mean = sum(a[0] for a in pi) / float(N_walker)
    long_s = []
    short_s = []
    for p in pi:
        if p[0] > walker_mean:
            long_s.append(p[:])
        else:
            short_s.append(p[:])
    walker_table = []
    for k in range(N_walker - 1):
        e_plus = long_s.pop()
        e_minus = short_s.pop()
        walker_table.append(((e_minus[0], e_minus[1], e_plus[1])))
        e_plus[0] = e_plus[0] - (walker_mean - e_minus[0])
        if e_plus[0] < walker_mean:
            short_s.append(e_plus)
        else:
            long_s.append(e_plus)
    if long_s != []:
        walker_table.append(((long_s[0][0], long_s[0][1], long_s[0][1])))
    elif short_s != []:
        walker_table.append(((short_s[0][0], short_s[0][1], short_s[0][1])))
    return N_walker, walker_mean, walker_table
def sample_cell_veto (active_cell):
    """determine the cell which raised the cell veto""
    # first sample the distance vector using Walker's algorithm
    i = random.randint (0, N_walker - 1)
    Upsilon = random.uniform (0.0, walker_mean)
    if Upsilon < walker_table[i][0]:
        veto_offset = walker_table[i][1]
    else:
        veto_offset = walker_table[i][2]
    # translate with respect to active cell
    veto_rate = Q_cell[veto_offset][0]
    vetoing_cell = translated_cell (veto_offset, active_cell)
    return vetoing_cell, veto_rate

N = 40
k_max = 3  # extension of periodic images.
chain_ell = 0.18  # displacement during one chain
L = 10  # number of cells along each dimension
density = N / 1.
cell_side = 1.0 / L

# precompute the cell-veto rates

# cell_boundary = []
cb_discret = 10  # going around the boundary of a cell (naive)
for i in range (cb_discret):
    x = i / float (cb_discret)
    cell_boundary += [(x*cell_side, 0.0), (cell_side, x*cell_side),
                      (cell_side - x*cell_side, cell_side),
                      (0.0, cell_side - x*cell_side)]

excluded_cells = [ del_x + L*del_y for del_x in (0, 1, L-1) \
                   for del_y in (0, 1, L-1) ]
Q_cell = []

for del_y in xrange (L):
    for del_x in xrange (L):
        k = del_x + L*del_y
        Q = 0.0
        # "nearby" cells have no cell vetos
        if k not in excluded_cells:
            # scan the cell boundaries of both active and target cells
            # to find the maximum of event rate
            for delta_a in cell_boundary:
                for delta_t in cell_boundary:
                    delta_x = del_x*cell_side + delta_t[0] - delta_a[0]
                    delta_y = del_y*cell_side + delta_t[1] - delta_a[1]
                    Q = max (Q, pair_event_rate (delta_x, delta_y))
            Q_cell.append ([Q, k])

Q_tot = sum (a[0] for a in Q_cell)
N_walker, walker_mean, walker_table = walker_setup (Q_cell)

# histogram for computing g(r)
hbins = 50
histo = np.zeros (hbins)
histo_binwid = .5 / hbins
hsamples = 0

# random initial configuration
particles = [(random.uniform(0.0, 1.0), random.uniform(0.0, 1.0))
    for _ in xrange(N)]

for iter in xrange(10000):
    if iter % 100 == 0:
        print iter

    # possibly exchange x and y coordinates for ergodicity
    if random.randint(0, 1) == 1:
        particles = [(y, x) for (x, y) in particles]

    # pick active particle for first move
    active_particle = random.choice(particles)
    particles.remove(active_particle)

    active_cell = cell_containing(active_particle)

    # put particles into cells
    surplus = []
    cell_occupant = [None] * L * L
    for part in particles:
        k = cell_containing(part)
        if cell_occupant[k] is None:
            cell_occupant[k] = part
        else:
            surplus.append(part)

    # run one event chain
    distance_to_go = chain_ell
    while distance_to_go > 0.0:
        planned_event_type = 'end-of-chain'
        planned_displacement = distance_to_go
        target_particle = None
        target_cell = None

        active_cell_limit = cell_side * (active_cell % L + 1)
        if active_cell_limit - active_particle[0] <= planned_displacement:
            planned_event_type = 'active-cell-change'
            planned_displacement = active_cell_limit - active_particle[0]

        delta_s = random_exponential(Q_tot)
        while delta_s < planned_displacement:
            vetoing_cell, veto_rate = sample_cell_veto(active_cell)
            part = cell_occupant[vetoing_cell]
            if part is not None:
                Ratio = pair_event_rate(part[0] - active_particle[0] - delta_s,
                                        part[1] - active_particle[1]) / veto_rate
                if random.uniform(0.0, 1.0) < Ratio:
                    planned_event_type = 'particle'
                    planned_displacement = delta_s
                    target_particle = part
                    target_cell = vetoing_cell
                    break

        delta_s += random_exponential(Q_tot)
# compile the list of particles that need separate treatment
extra_particles = surplus[:]
for k in excluded_cells:
    part = cell_occupant[translated_cell(k, active_cell)]
    if part is not None:
        extra_particles.append(part)

# naive version of the short-range code by discretization
delta_s = 0.0
short_range_step = 1e-3
while delta_s < planned_displacement:
    for possible_target_particle in extra_particles:
        # this supposes a constant event rate over the time interval
        # [delta_s:delta_s+short_range_step]
        q = pair_event_rate(possible_target_particle[0] - active_particle[0] - delta_s,
                            possible_target_particle[1] - active_particle[1])
        if q > 0.0:
            event_time = random_exponential(q)
            if event_time < short_range_step and delta_s + event_time < planned_displacement:
                planned_event_type = 'particle'
                planned_displacement = delta_s + event_time
                target_particle = possible_target_particle
                target_cell = cell_containing(target_particle)
                break
    delta_s += short_range_step

# advance active particle
distance_to_go -= planned_displacement
new_x = active_particle[0] + planned_displacement
active_particle = (new_x % 1.0, active_particle[1])

if planned_event_type == 'active-cell-change':
    ac_x = (active_cell_limit + 0.5*cell_side) % 1.0
    active_cell = cell_containing([ac_x, active_particle[1]])
    active_particle = (active_cell % L * cell_side, active_particle[1])

elif planned_event_type == 'particle':
    # remove newly active particle from store
    if target_particle in surplus:
        surplus.remove(target_particle)
    else:
        cell_occupant[target_cell] = None
    # put the previously active particle in the store
    if cell_occupant[active_cell] is not None:
        surplus.append(active_particle)
    else:
        cell_occupant[active_cell] = active_particle
active_particle = target_particle
active_cell = cell_containing(active_particle)

# restore particles vector for x <-> y transfer
particles = [active_particle]
particles += [part for part in cell_occupant if part is not None]
particles += surplus
# form histogram for computing radial distribution function \( g(r) \)
for \( k \) in range (len (particles)):
    for \( l \) in range (k):
        ibin = int (dist (particles[k], particles[l]) / histo_binwid)
        if ibin < len (histo):
            histo[ibin] += 1
    hsamples += 1

# compute \( g(r) \) from histogram
half_bin = .5 * histo_binwid
r = np.arange (0., hbins) * histo_binwid + half_bin
\( g_of_r \) = histo / density / hsamples * 2
\( g_of_r \) /= math.pi * ((r+half_bin)**2 - (r-half_bin)**2)
# save \( g(r) \)
np.savetxt ('cvmc-radial-distr-func.dat', zip (r, g_of_r))