Kinetic Monte Carlo simulations of two-dimensional pedestrian flow models

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Abstract

We employ an efficient list-based kinetic Monte Carlo (KMC) method to study two-way and four-way pedestrian flow models on two-dimensional (2D) lattices based on the exclusion principle and Arrhenius microscopic dynamics. This model implements stochastic rules for pedestrians' movements based on the configuration of the surrounding conditions of each pedestrian. Although the decision-making process of pedestrians is more complex and adaptive to dynamic conditions than vehicular flows, our rules can reflect the pedestrians' decisions of action such as moving forward, stopping to wait, lane switching, back stepping, etc. The simulation results of both two-way and four-way flows exhibit a state transition from freely flowing to fully jammed, as a function of initial density of pedestrians. At different states the relationships of density-flow and density-velocity are different from each other. The KMC simulations reported in this paper are compared with those from other well-known pedestrian flow models and the corresponding empirical results from real traffic.

1. Introduction

In the past few decades, traffic problems have been studied considerably in order to understand the mechanisms leading to traffic jams and improve design of traffic networks for efficient transportation systems. A large number of theoretical and computational models have been proposed to study traffic flows from the perspective of nonequilibrium statistical physics (see the review papers or books [1–9] and references therein). While the modeling of vehicular traffic has been undertaken intensively, the modeling on pedestrian flows has received less attention due to the fact that they are more complex and less predictable, which gives rise to a large variety of collective effects and self-organization phenomena that are not observed in vehicular flows. Therefore, only a few models can reproduce the empirical data accurately and it has become a fundamental task to model pedestrian dynamics (see the review papers or books [8–12]).
The models for pedestrian flows can be roughly divided into several categories: (i) microscopic discrete lattice models where a lattice site configuration with values 1 (pedestrian is present) and 0 (pedestrian is absent) combined with explicit rules for pedestrian movement on lattice sites is used to represent pedestrian flow; (ii) microscopic noninteger off-lattice models that treat pedestrians as particles and use ordinary differential equations (ODEs) to describe the motion of pedestrians with interactions depending on the distances between them; (iii) macroscopic fluid-dynamic and gas-kinetic models that treat the pedestrian flow as a compressible fluid formed by the pedestrians and use partial differential equations (PDEs, typically conservation laws) to relate the density and flux of pedestrians [13–19].

In the microscopic models above, attention is explicitly focused on individual pedestrians, and the interactions among them are determined by how nearby pedestrians influence each other’s movements. Among the off-lattice models, the social-force (SF) model [20–22] and the optimal velocity (OV) model [23,24] were proposed to provide a setup allowing for detailed interaction rules and mechanisms. In the SF model [20–22], the interactions between pedestrians are implemented by using the concept of a social force or social field, which represents the influence of other pedestrians, infrastructure, etc. Calibrations of the parameter sets and other modifications of the SF model using empirical data can be found in [25–28]. In [23], Nakayama, Hasebe, and Sugiyama generalized the OV model for vehicular flows to two dimensions for pedestrian flows and discussed the instability of pedestrian dynamics and pattern structure, and in [24] they extended their model by incorporating the attractive interaction between pedestrians.

Compared with the off-lattice models, lattice models are simpler to implement and are more amenable to numerical investigation. Therefore, lattice models, such as the cellular automata (CA) [29,30], have been widely used to represent traffic flow, in particular, vehicular traffic [5,31–37]. Recently, a look-ahead rule was used to model the effect of long-range traffic conditions in a CA model, which was then coarse-grained to derive a macroscopic PDE description with nonlocal interactions [38]. Extensions to multilane and multiclass traffic have also been developed [39,40]. An improved coarse-grained model at the ODE level has been discussed in [41]. Two different look-ahead rules in both one-dimensional (1D) and two-dimensional (2D) CA models were compared in [42]. On the other hand, CA models with empirical rules have also been used to simulate the pedestrian dynamics. Blue and Adler [43,44] have extended two-lane variants of the Nagel–Schreckenberg model [32] for the description of pedestrian flows. Fukui and Ishibashi (FI) [45,46] have studied bidirectional pedestrian flows in a long corridor. Nagatani and collaborators [47–50] have used variations of the FI model to investigate situations where a jamming transition can occur. In [51,52], the so-called floor field model was introduced by Schadschneider and collaborators, which has become a standard CA approach to pedestrian dynamics. In [53,54], Yue et al. have combined the idea of the FI model with that of the floor field model to propose the dynamic parameter models, which can obtain more realistic fundamental diagrams.

The main goal of this work is to study two-way and four-way pedestrian flow models on 2D lattices based on the exclusion principle and Arrhenius microscopic dynamics and to use the kinetic Monte Carlo (KMC) simulations [55] for improving computational efficiency due to its main feature—“rejection-free”. In both of these models pedestrians’ movement is described using stochastic rules based on the configuration of the surrounding conditions of each pedestrian. Our rules can reflect the pedestrians’ decisions of action such as moving forward, stopping to wait, lane switching, back stepping, etc. Numerically we employ the KMC algorithm to simulate the microscopic stochastic dynamics of the pedestrian flow based on the Arrhenius law with these rules. When the pedestrian dynamics features a finite number of distinct processes in configurational changes, we develop an efficient list-based KMC algorithm using fast search that can further improve computational efficiency compared to the general KMC method. On the other hand, the Metropolis Monte Carlo (MMC) method [56] is adopted in most of current CA models for vehicular flows and pedestrian flows. But the MMC method is a way of simulating an equilibrium distribution for a model, and trial steps are sometimes rejected because the acceptance probability is small, in particular when a system approaches the equilibrium, or the density of pedestrians is high. Therefore, we choose the KMC, which is more suitable for simulating the time evolution of the pedestrian systems.

To have a reasonable time scale in the KMC method, the model parameters (the characteristic time unit and the interaction strength) are calibrated against empirical results from real traffic. The behavior of discrete lattice models can vary drastically with respect to parameters in the model, and by calibrating the models discussed in this paper we ensure, in particular, that our numerical simulations can be adequately compared with other results in the literature. After calibration, the KMC simulations are used to quantitatively predict the time evolution of 2D pedestrian flows. Our results show that the rules induce asymmetry in the fundamental diagram, which changes from concave to convex. The simulation results of both two-way and four-way flows exhibit a state transition from freely flowing to fully jammed, as a function of initial density of pedestrians. At different states the relationships of density–velocity and density–flow are different from each other.

The rest of the paper is organized as follows. In Section 2, we introduce lattice models with pedestrians’ interaction rules. In Section 3, we describe the list-based KMC algorithm and its implementation. In Section 4, we provide a series of numerical simulations in various parameter regimes for two-way and four-way pedestrian flows, respectively. We state our conclusions in Section 5.

2. A lattice-based model

We discuss the construction of the discrete lattice model for 2D pedestrian flow in this section. For simplicity, the model is defined on a square lattice with $M \times M$ cells, where $M$ is the size. The configuration at each cell $x = (i,j)$ for $1 \leq i,j \leq M$ is defined by an index $\sigma_x$:

$$\sigma_x = \begin{cases} 1 & \text{if a pedestrian occupies cell } x, \\ 0 & \text{if the cell } x \text{ is empty.} \end{cases}$$  

(1)
and the state of the system is represented by the configuration space \([0, 1]^{M^2}\). Transitions in the state of this system represent the pedestrian movements, which obey the rules of an exclusion process [57]: two nearest-neighbor lattice cells exchange values in each transition and pedestrians cannot occupy the same cell. In addition, pedestrians are allowed to move into only one of the nearest-neighbor cells in one transition. Here, we consider the Moore neighborhood which consists of eight nearest-neighbor cells [29, 30]. For example, the case for a pedestrian at cell \(x = (i, j)\) moving north to \(y = (i, j + 1)\) is of the form (see Fig. 1(a))

\[
\{\sigma_x = 1, \sigma_y = 0\} \rightarrow \{\sigma_x = 0, \sigma_y = 1\}.
\]

The transition rate depends on spatial Arrhenius-type interactions with a one-sided interaction and traffic situation around the moving pedestrian. This is similar to the spin-exchange Arrhenius dynamics in which the simulation is driven based on the energy barrier a particle has to overcome in changing from one state to another [38, 40]. During a spin-exchange between nearest neighbor sites \(x\) and \(y\), the system will allow the index \(\sigma_x\) at location \(x\) to exchange sign with the one at \(y\). This is interpreted as a pedestrian move from \(x\) to \(y\) with the rate given by the Arrhenius relation:

\[
r(x, y, \sigma) = \begin{cases} 
\omega_0 \exp[-E(x, y)], & \text{if } \sigma_x = 1, \sigma_y = 0, \\
0, & \text{otherwise},
\end{cases} (2)
\]

where the prefactor \(\omega_0 = 1/\tau_0\) corresponds to the pedestrian moving frequency and \(\tau_0\) is the characteristic or relaxation time. The moving energy barrier \(E(x, y)\) is assumed to depend only on the local environment of the pedestrian under consideration and it is given by

\[
E(x, y) = E_0(x) + E_p(x, y),
\]

where \(E_0(x)\) is the external potential associated with the site binding of the pedestrian, which could vary in both space and time to account for spatial and temporal traffic situations, such as rush hour traffic, local weather anomalies, etc. [40]. In this study we set \(E_0(x) = 0\). The parameter \(E_p(x, y)\) is the pedestrian interaction strength, which depends on the pedestrian’s type (i.e., his/her destination) and his/her moving direction from \(x\) to \(y\). Based on the formula (2), we can see that the smaller is the energy barrier \(E_p\), the larger is the transition rate \(r\).

Here we take a northbound pedestrian (▲) at the cell \(x = (i, j)\) as an example to illustrate the dynamic rules and the parameter \(E_p(x, y)\). As shown in Fig. 1(b), when the northbound pedestrian moves straightforwardly from \(x = (i, j)\) to the north neighboring cell \(y = (i, j + 1)\), we take \(E_p = E_d\); if the northbound pedestrian moves in the northeast or northwest direction to \(y = (i \pm 1, j + 1)\), we take \(E_p = E_b\). Since the destination of the northbound pedestrians is the north boundary of the square lattice, the pedestrian prefers to choose the cells in the direction towards the north boundary in order to arrive there with a route as short as possible. Therefore, we should make \(E_a < E_b\) so that the rate \(r_a > r_b\), i.e., the probability of moving straightforward is larger than that of moving into north-diagonal cells. Otherwise, if \(E_a = E_b\), the pedestrian will move into one of the upper three cells in front of him/her with equal probability and his/her path will be a zigzag line instead of a straight line.

If the northbound pedestrian chooses to move horizontally into the left or right cell at \(y = (i \pm 1, j)\), he/she will not be able to get any closer to the destination. For this case, we take \(E_p = E_c > E_b\) so that the rate \(r_c < r_b\). Similarly, if the northbound pedestrian chooses to move in the southeast/southwest directions to \(y = (i \pm 1, j - 1)\) or backward to \(y = (i, j - 1)\), we take \(E_p = E_d\) or \(E_c\), respectively. All five parameters should satisfy that \(E_a < E_b < E_c < E_d < E_e\). In summary, for a northbound pedestrian (▲) moving from \(x = (i, j)\) to one of eight nearest-neighbor cells at \(y\), the interaction strength is given by

\[
E_p(x, y) = \begin{cases} 
E_a, & \text{if } y = (i, j + 1), \\
E_b, & \text{if } y = (i \pm 1, j + 1), \\
E_c, & \text{if } y = (i \pm 1, j), \\
E_d, & \text{if } y = (i \pm 1, j - 1), \\
E_e, & \text{if } y = (i, j - 1).
\end{cases} (3)
\]

Fig. 1. Schematic representation of pedestrian dynamic rules and parameters. (a) The movement field of a northbound pedestrian, who may stay at the core cell or move into one of the eight nearest neighboring cells. (b) The interaction strength parameters for the pedestrian to move into the corresponding cells.
In the same way, we may define the interaction strength $E_p$ for the other three species of pedestrians. Then all pedestrians’ moving events can be classified into six folds according to the corresponding values of $E_p$ in (3) for moving in different directions or the case of staying at the core cell, as shown in Fig. 1(b).

In the two-way pedestrian flow model, we consider two species of pedestrians: the eastbound (▲) and northbound (▲). In the four-way pedestrian flow model, we use four species of pedestrians: the eastbound (▲), westbound (▲), southbound (▼) and northbound (▲). For the southbound and northbound pedestrians, periodic boundary conditions are applied at the south and north boundaries. For example, if a northbound pedestrian moves out of the north boundary, he/she will reenter the lattice domain from the south boundary. Here, since we consider the situation where two roads cross, the southbound and northbound pedestrians are inhabited from crossing the east and west boundaries, where closed boundary conditions are adopted. Similarly, for the eastbound and westbound pedestrians, periodic boundary conditions are applied at the east and west boundaries, and the closed boundary conditions are adopted at the south and north boundaries. Therefore, the number of pedestrians in the system is conserved during simulations. Suppose that $N_s$ is the number of the northbound pedestrians in the system. The density of the northbound pedestrians is given by $\rho_s = N_s / M^2$. In the two-way model, we will focus on the symmetric cases with equal densities of the eastbound and northbound pedestrians, i.e., $\rho_e = \rho_s = \rho / 2$, where $\rho$ is the total density of the pedestrians. In the four-way model, we also focus on the symmetric cases with $\rho_e = \rho_s = \rho = \rho / 4$.

To summarize, the following parameters need to be given for the stochastic simulations with the pedestrian dynamic rules: (i) the characteristic or relaxation time $\tau_0$; (ii) the pedestrian interaction strength parameters $E_a$, $E_b$, $E_c$, $E_d$, $E_e$.

3. The kinetic Monte Carlo method

We apply the kinetic Monte Carlo (KMC) method to the above lattice model to investigate the evolution of the pedestrian system. We choose the KMC instead of the Metropolis Monte Carlo (MMC) method [56] since in the MMC, trial steps are sometimes rejected because the acceptance probability is small, in particular when a system approaches the equilibrium, or the density of pedestrians is high. The KMC method that we adopt here is related to the method proposed by Bortz, Kalos, and Lebowitz as a speedup to the MMC method for simulating the evolution of Ising models [55]. A main feature of the KMC algorithm is that it is “rejection-free”. In each step, the transition rates for all possible changes from the current configuration are calculated and then a new configuration is chosen with a probability proportional to the rate of the corresponding transition. Since the interaction is short ranged within the nearest-neighbors, there is only a small number of local environments that need to be changed due to the previous transition.

The KMC algorithm is built on the assumption that the model features $N$ independent Poisson processes (corresponding to $N$ moving events on the lattice) with transition rates $r_i$ in (2) that sum up to give the total rate $R = \sum_{i=1}^{n} r_i$. In simulations with a finite number of distinct processes it is more efficient to consider the groups of events according to their rates [58–60]. This can be done by forming lists of the same kinds of events according to the values of $E_p$ in (3). As we mentioned above, there are five different values of $E_p$ for moving in different directions and one case of staying at the core cell. Therefore, we can put the total $N$ events into $L$ lists ($L = 6$), labeled by $l = 1, \ldots, L$. All processes in the $l$th list have the same rate $r_l$. We denote the number of processes in this list by $n_l$, which is called the multiplicity, and we have $N = \sum_{l=1}^{L} n_l$. To each list we assign a partial rate $R_l = n_l r_l$, and a relative probability $P_l = R_l / R$. Then the total rate is given by $R = \sum_{l=1}^{L} n_l r_l$. A fast list-based KMC algorithm at each step based on the grouping of events is given as follows.

List-based KMC algorithm

Step 1. Generate a uniform random number $\xi_1 \in (0, 1)$ and decide which process will take place by choosing the list index $s$ such that

$$\sum_{l=1}^{s-1} \frac{R_l}{R} < \xi_1 \leq \sum_{l=1}^{s} \frac{R_l}{R} \quad (4)$$

Step 2. Select a realization of the process $s$. This can be done with the help of a list of coordinates for each kind of event, and an integer random number $\xi_2$ in the range $[1, n_s ]$. $\xi_2$ is generated and the corresponding member from the list is selected.

Step 3. Perform the selected event leading to a new configuration.

Step 4. Use $R$ and another random number $\xi_3 \in (0, 1)$ to decide the time it takes for that event to occur (the transition time), i.e., the nonuniform time step $\Delta t = - \log(\xi_3) / R$.

Step 5. Update the multiplicity $n_i$, relative rates $R_i$, total rate $R$ and any data structure that may have changed due to that event.

4. Numerical experiments

We next investigate two-way and four-way pedestrian flows in various parameter regimes with the numerical method developed in the previous section. Following [9,61], we set the physical size of each cell to $0.4 \times 0.4$ m$^2$, which allows one to keep a minimal distance to others in order to avoid bumping into them. This is consistent to the fact that maximal densities
of about 6 pedestrians/m² can be observed in dense crowds [9]. For a pedestrian who has an average speed of ≈ 1.2 m/s, an estimate of time to cross a cell is given by

\[ \Delta t_{\text{cell}} = \frac{0.4 \text{ m}}{1.2 \text{ m/s}} = \frac{1}{3} \text{s}. \]  

(5)

In a free-flow regime, we expect all pedestrians to move at their desired speed that is set to 3 cells/s (≈ 1.2 m/s). This is accomplished by setting the characteristic time \( t_0 = 1/3 \text{s} \), and then \( \sigma_0 = 3 \text{s}^{-1} \). In fact, due to the inherent stochasticity in the simulations, sometimes pedestrians may move faster or slower than the average speed.

As there are five interaction strength parameters \( E_a \) to \( E_e \) to be explored, for simplicity, we take a linear fixed relationships between them, which is similar to the choice of piecewise constants for short-range local interactions in the look-ahead rules of modeling traffic flow [38,42]. We take \( E_a = 0 \) and therefore the rate \( r(x, y, \sigma) = \omega_0 \exp(0) = \omega_0 \), thus with the maximum probability of moving straightforward towards the pedestrian’s destination. In the following Sections 4.1, 4.2 and 4.4, we take \( E_b = 2.0, E_c = 4.0, E_d = 6.0 \), and \( E_e = 8.0 \) to show some typical configurations and fundamental diagrams of the pedestrian flows and compare results with empirical data. In the Section 4.3, we take different values of \( E_b \) from 1.0 to 3.0 with fixed relationships \( E_c = 2E_b, E_d = 3E_b, \) and \( E_e = 4E_b \) to compare fundamental diagrams of the pedestrian flows. It is possible to explore different and more complex relationships between these parameters close to the realistic situations. Given the real data, one may employ the deep learning tool in the form of an energy method like the Boltzmann machine to calibrate the interaction parameters with respect to a set of specific pedestrian types in the study [62].

4.1. Numerical results of configurations

Here, we perform a series of simulations for different pedestrian densities \( \rho \) with various values of the lattice size \( M \). At the beginning of each simulation, the pedestrians are randomly distributed on the lattice. The results exhibit a state transition from the free-flow regime to the completely jammed regime as the pedestrian density increases.

Fig. 2 shows four typical configurations of the two-way pedestrian flow on an \( M \times M \) lattice of size \( M = 50 \). Fig. 2(a) displays a configuration below the transition, i.e., the free-flow state with a low pedestrian density \( \rho = 0.1 \), where the pedestrians are distributed randomly and homogeneously. Fig. 2(b) shows a partially jammed state with \( \rho = 0.3 \) above the transition, where some jams have formed at the east and north boundaries, but they are not completely blocking the two boundaries so that some pedestrians can still pass through the boundaries. Another partially jammed state with \( \rho = 0.4 \) is shown in Fig. 2(c). Here a big jam completely blocks path of all northbound (▲) pedestrians, but there is a channel formed at the lower part of the lattice for some eastbound (●) pedestrians to pass. Fig. 2(d) shows a high-density, completely jammed state with \( \rho = 0.6 \), where the jammed pedestrians assemble in the right and upper parts of the lattice and there is no channel formed for pedestrians to pass. The boundary between the two types of pedestrians in the jam is irregular. The intrinsic stochasticity of the dynamics triggers the onset of jamming and the phenomenon of complete jamming through self-organization as well as the final jammed configurations. We note that the configurations using other values of the lattice size \( M \) produce similar results, which are not shown for the brevity of the presentation.

Fig. 3 shows four typical configurations of the four-way pedestrian flow with the size \( M = 50 \). Fig. 3(a) displays a configuration of the free-flow state with a low pedestrian density \( \rho = 0.08 \). Fig. 3(b) shows a partially jammed state with \( \rho = 0.2 \), where small jams have formed not only at the corners of the lattice, but also inside the domain. A completely jammed state with \( \rho = 0.5 \) is shown in Fig. 3(c), where pedestrians get stuck at the four boundaries of their destinations with an empty space formed at the center of the lattice. Fig. 3(d) shows another completely jammed state with a high-density \( \rho = 0.7 \). In this state, the system has very short time to self-organize, and instead of one big hole in the center, we observe several small holes appearing simultaneously on the lattice. The pedestrians are jammed at four sides of each hole towards their destinations, respectively.

4.2. Numerical comparisons of flows with different sizes

Similar to vehicular traffic, the main characteristic quantities for the description of pedestrian streams are flow and density. To identify the parameter range of the state transition, we make a series of KMC simulations with different pedestrian densities ranging from \( \rho = 0.01 \) to \( \rho = 0.99 \) until the same final time (2 h). In the following we show the fundamental diagrams of the density–flow and density–velocity relationships, and compare the results of the two-way and four-way pedestrian flows.

For each simulation we compute long-time averages of the flow \( \langle F \rangle \) in number of pedestrians crossing a fixed location of a facility per hour per lane and obtain the ensemble-averaged velocity \( \langle v \rangle \) in cells per second by averaging the velocities over all pedestrians. For example, in the two-way model, the average flow \( \langle F \rangle \) of pedestrians is measured as the sum of the eastbound pedestrians passing through the east boundary and the northbound pedestrians passing through the north boundary minus the sum of the eastbound pedestrians moving backward through the west boundary and the northbound pedestrians moving backward through the south boundary during one hour, divided by the system size, \( M \). Similarly, in the four-way model, the average flow \( \langle F \rangle \) is measured as the total sum of four types of pedestrians passing through the boundaries of their destinations minus the sum of all four types of pedestrians moving backward through the boundaries during one hour, divided by \( M \). Moreover, for every value of \( \rho \), we report results averaged over ten simulations with different random number seeds.
Fig. 2. (Color online) Typical configurations of the two-way pedestrian flow on an $M \times M$ lattice of size $M = 50$. The eastbound and northbound pedestrians are represented by red (●) and black (▲), respectively. In all KMC simulations, we take the interaction strengths $E_a = 0$, $E_b = 2.0$, $E_c = 4.0$, $E_d = 6.0$, $E_e = 8.0$ and the final time is 2 h. (a) A free-flow state with a low pedestrian density $\rho = 0.1$. (b) A partially jammed state with $\rho = 0.3$. (c) A partially jammed state with $\rho = 0.4$. (d) A high-density, completely jammed state with $\rho = 0.6$.

For critical phenomena of state transition, it is expected that the size of the system plays an important role. Therefore, we also analyze the effects of the lattice size $M$ on the pedestrian flows in Fig. 4, where results of five system sizes from $10 \times 10$ to $100 \times 100$ are presented in each panel. All curves exhibit state transitions between the free-flow state and the jammed state. Here, certain characteristics are shared by most fundamental diagrams that have been obtained empirically, e.g., a linear increase of the flow at low densities, a single maximum of the flow, and an asymmetry towards smaller densities. These features are similar to the characteristics of fundamental diagrams of vehicular traffic [9,10].

As shown in Fig. 4(a) and (b), in the free-flow regime the value of $\langle F \rangle$ increases as the pedestrian density $\rho$ increases, and reaches its maximum at the critical value, $\rho_{crit}$. Beyond that point, the state transition starts and the flow drops down to zero as all pedestrians are stopped. On the other hand, Fig. 4(c) and (d) show that in the free-flow regime the ensemble-averaged velocity $\langle v \rangle$ decreases approximately linearly from the maximum speed of 3 cells per second (i.e., $\approx 1.2$ m/s) as $\rho$ increases and the chance of interaction between pedestrians gets higher. When $\rho$ is larger than the critical point $\rho_{crit}$, the average velocity also drops down quickly to zero and the density–velocity curve is negative exponential. This linear relationship follows the Greenshields model [63] and the negative exponential relationship belongs to the Underwood model [64]. We also observe that as the system size $M$ increases, both the value of $\rho_{crit}$ and the maximum value of flow tend to decrease.
Fig. 3. [Color online] Typical configurations of the four-way pedestrian flow on an $M \times M$ lattice of size $M = 50$. The pedestrians are represented by red ($\uparrow$) for the eastbound, blue ($\gets$) for the westbound, cyan ($\Downarrow$) for the southbound, and black ($\Uparrow$) for the northbound, respectively. In all KMC simulations, we take the interaction strengths $E_a = 0$, $E_b = 2.0$, $E_c = 4.0$, $E_d = 6.0$, $E_e = 8.0$ and the final time is 2 h. (a) A free-flow state with a low pedestrian density $\rho = 0.08$. (b) A partially jammed state with $\rho = 0.2$. (c) A completely jammed state with $\rho = 0.5$. (d) A high-density, completely jammed state with $\rho = 0.7$.

However, as in the Biham–Middleton–Levine model for the vehicular traffic in cities [33], currently we are not able to determine whether $\rho_{\text{crit}}$ converges to a finite value or to zero in the infinite system limit.

We note that in the two-way model, when $\rho > \rho_{\text{crit}}$, the value of flow $\langle F \rangle$ varies according to the jamming states and therefore the curves of the density–flow relationship fluctuate (see Fig. 4(a); recall that each result on the curves was already averaged over ten simulations with different random number seeds. Otherwise, the curves of single runs will have more fluctuations, which are not shown). This is because that in the free-flow regime there is no jam or only small jams exist, which has little effect on the increase of flow $\langle F \rangle$ (see Fig. 2(a)). But when $\rho > \rho_{\text{crit}}$, there are different types of jamming states. For example, in the partially jammed states shown in Fig. 2(b) and (c), there are channels formed on the lattice for certain types of pedestrians to pass. In these states, the value of flow $\langle F \rangle$ has something to do with the width of the channels. The wider the channels are, the larger the value is. Fig. 2(d) shows that the completely jammed state has no channel formed for pedestrians to pass and suppresses the pedestrian flows and their velocities.

As shown in Fig. 4(b) for the four-way model, both the values of the critical density $\rho_{\text{crit}}$ of the transition and the maximum values of the flow are smaller than the corresponding values in the two-way model with the same size $M$. When $\rho > \rho_{\text{crit}}$,ing.
Fig. 4. (Color online) Comparison results of the pedestrian flow model with five different system sizes from $M = 10$ to $M = 100$. In all KMC simulations, we take the interaction strengths $E_a = 0$, $E_b = 2.0$, $E_c = 4.0$, $E_d = 6.0$, $E_e = 8.0$ and the final time is 2 h. For every value of $\rho$ and $M$, we report results averaged over ten simulations with different random number seeds. (a),(b): Long-time averages of the density–flow relationship of pedestrians. (c),(d): Ensemble-averaged velocity of pedestrians versus the density $\rho$. (a),(c): Results of the two-way pedestrian flow. (b),(d): Results of the four-way pedestrian flow.

Both the values of the flow $\langle F \rangle$ and the ensemble-averaged velocity $\langle v \rangle$ decrease more slowly with increasing $\rho$ than those values do in the two-way model (see Fig. 4(b) and (d)). Moreover, the fluctuations in the curves are smaller than those in the two-way model since the jams are gradually formed as $\rho$ increases and there are no channels formed (see Fig. 3(c) and (d)). The reason is that in the two-way model, there are only two types of pedestrians moving in perpendicular directions (e.g., the eastbound and northbound in Fig. 2). The movement of one type of pedestrians affects the other type from the perpendicular direction, as if one type of pedestrians “push” the other type to their closed boundary (i.e., the eastbound pedestrians to the north boundary, or the northbound pedestrians to the east boundary). Since the pedestrians cannot pass through their closed boundary, they accumulate there and block the path of the other type of pedestrians. If both boundaries of their destinations are completely blocked as shown in Fig. 2(d), the values of flow and velocity are extremely small or zero. If only one boundary is completely blocked and the other one is partially blocked, a channel can form as shown in Fig. 2(c), which allows a certain amount of flow and velocity. In the four-way model, each type of pedestrians is affected by the other three types from the opposite direction and the two perpendicular directions at their left and right sides. Since each type of pedestrian flows has the same density, the two effects of the flows from their left and right sides may cancel out. Therefore, most of jams are formed mainly due to the encountering flows with opposite directions and it is more difficult to form channels than the two-way model does. Hence, the fluctuations in the curves of the four-way model are much smaller.

4.3. Numerical comparisons of flows with different interaction strengths

Next, we analyze the effects of the pedestrian interaction strengths $E_p$ on the flows in Fig. 5. For simplicity, we take $E_a = 0$ and different values of $E_b$ from 1.0 to 3.0 with fixed relationships $E_c = 2E_b$, $E_d = 3E_b$, and $E_e = 4E_b$. All curves exhibit state transitions between the free-flow state and the jammed state. However, Fig. 5 shows that the two-way and four-way models produce different results in both diagrams of density–flow and density–velocity relationships.

As shown in Fig. 5(a) and (c) for the two-way model, the density–flow and density–velocity curves clearly display that the region of free flow in all five cases with different values of the parameter $E_b$ persists up to almost the same critical density $\rho_{\text{crit}} = 0.18$, i.e., $50^2 \times 0.18 = 450$ pedestrians on the lattice of 400 m$^2$ (≈1.125 pedestrians per m$^2$). In all cases, the flow $\langle F \rangle$ increases as the pedestrian density $\rho$ increases until $\rho_{\text{crit}}$ when the transition happens. The ensemble-averaged velocity $\langle v \rangle$ decreases approximately linearly from the maximum speed of 3 cells per second (i.e., ≈1.2 m/s) with the increase of $\rho$. After the transition, both the values of the flow and the ensemble-averaged velocity drop down quickly and eventually decay to zero. Moreover, the maximum value of the flow tends to increase as $E_b$ increases to 2.5. But when $\rho > \rho_{\text{crit}}$, for the same value of $\rho$, both the values of the flow and the average velocity decrease with increasing $E_b$. The reason is that
Fig. 5. (Color online) Comparison results of the pedestrian flow model with five different values of the interaction strength $E_b$ from 1.0 to 3.0 with $E_a = 0$ and fixed relationships $E_c = 2E_b$, $E_d = 3E_b$, and $E_e = 4E_b$. In all KMC simulations, we take the same size $M = 50$ and the final time is 2 h. For every value of $\rho$ and $E_b$, we report results averaged over ten simulations with different random number seeds. (a), (b): Long-time averages of the density–flow relationship of pedestrians. (c), (d): Ensemble-averaged velocity of pedestrians versus the density $\rho$. (a), (c): Results of the two-way pedestrian flow. (b), (d): Results of the four-way pedestrian flow.

for larger $E_b$, the pedestrians prefer to move straightforward towards their destinations since the probabilities of moving in other directions are much smaller, which produces completely jammed cases more often.

On the other hand, in Fig. 5(b) for the four-way model, we observe that both the value of $\rho_{\text{crit}}$ of the transition and the maximum value of the flow $\langle F \rangle$ tend to decrease as the parameter $E_b$ increases. After the flow reaches the maximum, it decreases slowly. Fig. 5(d) shows that the ensemble-averaged velocity $\langle v \rangle$ decreases slowly with the increase of $\rho$ before the transition. After that, the average velocity drops down quickly and eventually decays to zero. In particular, in the case of $E_b = 3.0$, the average velocity decreases quickly almost from the beginning since the value $\rho_{\text{crit}}$ is very small in this case.

In summary, from Figs. 4 and 5, it seems that for the two-way model, the system size $M$ plays a more important role in finding the critical density $\rho_{\text{crit}}$ of the transition than the pedestrian interaction strength $E_b$ does. But for the four-way model, both $M$ and $E_b$ have the effects on finding $\rho_{\text{crit}}$.

4.4. Numerical comparisons with empirical data

Finally, we compare the simulation results of the fundamental density–flow and density–velocity relationships with the empirical data shown in [65] for various types of infrastructure, flow composition, etc. fitted from the data in Fruin [66], Weidmann [67,68], Virkl and Elayadath [69], Older [70], Sarkar and Janardhan [71] and Tanariboon et al. [72]. For the comparison shown in Fig. 6, we adopt the units used in [65]: flow in peds/s/m, velocity in m/s, and density in peds/m$^2$. As we set the physical size of each cell to $0.4 \times 0.4 = 0.16$ m$^2$, there are about six pedestrians per square meter (peds/m$^2$).

Therefore, when the density reaches $\rho = 1.0$ in our simulations, all the cells on the lattice are occupied by pedestrians, which is equivalent to 6 peds/m$^2$ in real situations [9,61]. Meanwhile, we set the pedestrians’ desired speed to 3 cells/s, which corresponds to $\approx 1.2$ m/s and is in the range of pedestrians’ average moving speed between 1.1 m/s (leisure) and 1.6 m/s (business) [9].

In Fig. 6, we use two simulation results with the system size $M = 10$ and the interaction strengths $E_a = 0$, $E_b = 2.0$, $E_c = 4.0$, $E_d = 6.0$, $E_e = 8.0$: one case for the two-way model from Fig. 4(a) and (c) and the other case for the four-way model from Fig. 4(b) and (d). We can see that both the average flow $\langle F \rangle$ and the ensemble-averaged velocity $\langle v \rangle$ in the two-way simulation result have good match with some empirical data as the density $\rho$ increases. The four-way simulation result matches the empirical data only when the density is low. As $\rho$ increases, the result deviates from the empirical data. But this result at least reflects the transition trends of empirical data as $\rho$ increases from the low-density to high-density regimes.

The deviations between the simulations and the empirical data may be due to the simplification of the discrete cellular automata model, which allows the pedestrians move in only eight directions and cannot fully represent the continuity
Fig. 6. (Color online) Comparison results of the two-way (black circles) and four-way (red crosses) pedestrian flows with empirical data from [65]. Both of simulation cases are with the system size $M = 10$ and the interaction strengths $E_a = 0$, $E_b = 2.0$, $E_c = 4.0$, $E_d = 6.0$, $E_e = 8.0$. (a) The density–flow relationship of pedestrians. (b) The density–velocity relationship of pedestrians.

of pedestrians’ movement and limit their freedom. Therefore, when the pedestrian system is in the high-density regime, especially for the four-way model, different types of pedestrians interact more frequently and form completely jammed states more often. Then the flow and velocity in the four-way model are considerably lower than the empirical data. Meanwhile, the current model treats the pedestrians as individual agents with the same characteristics and ignores the diversity of pedestrians in reality, such as differences in walking speed, purpose, age, gender, etc [9]. Moreover, we propose our lattice model in a closed system and take the periodic and closed boundary conditions without external interference, while in real situations pedestrian flows may be affected by many external factors. Therefore, there are some deviations between our simulation results and the empirical data.

We also emphasize that even the empirical data shown in Fig. 6 differ considerably from each other. As Seyfried et al. pointed out in [73], several explanations for these deviations among the empirical data may include cultural and population differences [74], differences between uni- and multidirectional flow [75,76], short-ranged fluctuations [76], influence of psychological factors given by the incentive of the movement (commuters, shoppers) [77]. The last but not the least, the way of measurements of the empirical data in experiments may also be responsible for the deviation in the literature. Therefore, it is necessary to have more reliable data that can be used for validation and calibration of computational pedestrian models.

5. Conclusions

We have used the kinetic Monte Carlo (KMC) method for a 2D lattice model to study the two-way and four-way pedestrian flows. Our work is motivated by the growing need to understand mechanisms leading to traffic jams and develop quantitative approach to the optimal design of pedestrian facilities and the evaluation of escape routes. The cellular automata pedestrian flow models considered here incorporate stochastic rules for the movement of pedestrians and the interactions between them.

To simulate the time evolution of the pedestrian system, we developed an efficient list-based KMC algorithm using fast search that can further improve computational efficiency. In the KMC method, the dynamics of pedestrians is described in terms of the transition rates corresponding to possible configurational changes of the system, and then the corresponding time evolution of the system can be expressed in terms of these rates. The KMC simulations relied on the calibration of model parameters: the characteristic time $\tau_0$ and the pedestrian interaction strengths $E_a$, $E_b$, $E_c$, $E_d$, $E_e$. Then we use the KMC simulations to quantitatively predict the time evolution of two-way and four-way pedestrian flows. While the Metropolis Monte Carlo (MMC) method is a way of simulating an equilibrium distribution for a model, the KMC is more suitable for
simulating the time evolution of the pedestrian systems. Moreover, since the KMC algorithm is “rejection-free”, we choose the KMC as one of our contributions in terms of computational efficiency.

For both of the two-way and four-way pedestrian flows, we obtained fundamental diagrams with qualitatively meaningful flows which display several observed traffic states. It is well-known that the fundamental diagram of density–flow is skewed to the left in realistic traffic measurements and it changes from concave to convex [7]. Our simulations capture this phenomenon of asymmetry of the fundamental diagram. The numerical results of both flow models exhibit a state transition from freely flowing to fully jammed, as a function of the initial density of pedestrians. But comparison of the results of both flows with the same lattice size \( M \) shows that the two models produce different density–flow and density–velocity diagrams. Moreover, the simulation result of the two-way flow model has better match with the empirical data than the four-way flow model does.

Since our main goal is to compare the results of the two-way and four-way pedestrian flows, we propose our lattice models in a closed system and take the periodic and closed boundary conditions to keep the number of pedestrians and the density constant in a single simulation. Therefore, we have not applied our models to simulate some more complex nonstationary features, such as oscillations at bottlenecks in normal situations and blocked states produced in panic situations. It is possible to improve our 2D model further in the following directions. We can include entrances and exits in the model by adding dynamics mechanisms such as adsorption and desorption. We also need to consider nonsymmetric cases with unequal densities of different types of pedestrians. More complicated models addressing these aspects will be explored in the future.

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**References**


