On the Dynamics of Interacting Agents on an Ising Lattice

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Abstract— **A system of multiple agents is considered which at random times change their discrete states on an Ising lattice as a results of their internal interactions and possibly some external control. For certain applications such as directed self-assembly of charged particles, the stochastic dynamics of such interacting agents is represented by a master equation, or equivalently, by a continuous-time Markov chain. The dimension of this master equation is typically large and numerically intractable, since it grows combinatorially with the lattice size. This paper presents two alternative models at signif cantly lower complexity growing polynomially with the size of Ising lattice. These models describe the interactive dynamics of the agents by two different classes of coupled stochastic differential equations driven by doubly stochastic Poisson processes (Cox processes).**

I. Introduction

This paper presents two novel stochastic models describing the dynamics of systems of discrete-state interacting agents. To visualize such systems, consider the 2D lattice in Fig. 1(a) with L lattice sites occupied by $K < L$ unlabeled, identical particles, and no more than one particle in each site. Suppose these particles interact with each other, and as a result, they move from one site to another at random points in continuous time. This paper aims to develop classes of stochastic models to describe the dynamics of these interacting particles, i.e., to characterize the temporal evolution of their placement in the lattice sites.

In addition to interactions between the particles, external controls and disturbances can effectively alter their dynamics. As an illustrative example, consider a directed self-assembly process [1]–[8] schematically described in Fig. 1(b). In this process, a number of charged particles (e.g., DNA tiles) move between the sites of a planar square lattice under the electric f eld generated by other particles and a set of electrodes f xed at specif c points of the lattice (marked in Fig. 1(b) by small circles). By changing the electric potentials of the electrodes properly in time, the dynamics of particles is controlled to evolve their random initial distribution in Fig. 1(a) toward a desired geometry in Fig. 1(b). Certainly, design of a suitable control to achieve this goal requires a reliable model for the dynamics of the charged particles.

Besides directed self-assembly, many physical phenomena such as ferromagnetism are studied using Ising models rooted in statistical mechanics [9]. An Ising model is a mathematical description of a physical phenomenon that involves multiple interacting particles living in an Ising lattice of the nature

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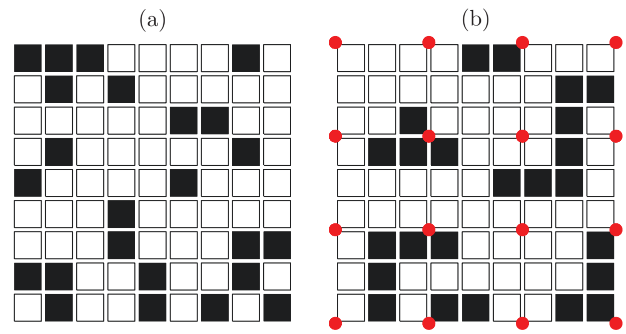

Fig. 1. Square Ising lattice in 2D: (a) 24 particles occupying 81 lattice sites with at most 1 particle at each site; (b) via a directed self-assembly process, a desired geometry is formed, starting from a random initial distribution of the particles. The small circles in (b) represent 16 electrodes through which an electric f eld is produced to control the dynamics of the charged particles.

shown in Fig. 1. Of course, an Ising lattice is not necessarily a 2D space similar to Fig. 1: depending on application, it can be a 1D, 2D, or 3D space.

This paper, on the other hand, adopts the notion of Ising lattice only as a means to visualize the state space of a system of discrete-state interacting agents, without referencing a specif c physical phenomenon. Hence, the more abstract term "agent" replaces the physical term "particle," and L sites of an Ising lattice are interpreted as the discrete state values of a single agent out of K unlabeled, identical, interacting agents. Then, an Ising lattice in the context of this paper can have any dimension and geometry, as long as it can visualize L sites to accommodate $K < L$ particles.

To characterize the dynamics of interacting particles on an Ising lattice, *master equation* is a common tool, adopted for instance, in directed self-assembly [10]–[14]. To implement a master equation, a probability is assigned to each possible conf guration of K particles occupying L lattice sites, and the temporal evolution of the assigned probabilities is described by a set of homogeneous linear differential equations, known in their vector form as master equation. A master equation indeed describes the evolution of probability distribution in a continuous-time Markov chain (CTMC). Therefore, the use of a master equation is equivalent to representing dynamics on an Ising lattice with a CTMC.

Although master equation is a physically justif ed model for many applications, it can be hard to use mathematically, since its dimension combinatorially increases with the size of the Ising lattice. For example, in directed self-assembly of 50 particles on a 20×20 square lattice, the dimension of master equation will be in the order of 1.7×10^{64}. Some efforts have been spent on simplifying the solution of large-scale master equations [15]; however, the proposed methods do not seem capable of coping with the dimensions as large as 1.7×10^{64}.

The goal of this paper is to break down the combinatorial dimension of the master equation by replacing its associated gigantic CTMC with a set of coupled CTMCs of affordable dimensions. Toward this goal, two different stochastic models are proposed, both relying on the concept of CTMC. In the first model, each interacting agent living on an Ising lattice is represented by a CTMC with a state space including all sites of the lattice. The interaction between the agents is expressed then by rendering the transition rate (infinitesimal generator) matrix of each CTMC dependent on the state of other agents. In the second proposed model, a binary CTMC is assigned to each lattice site to record the presence or absence of an agent in that specific site. Similar to the first model, the transition rate matrix of each binary CTMC is made dependent on the state of other sites. It is shown in the paper that both models are equivalent to a high dimensional CTMC with some sparse structure in its transition rate matrix. Physical justification of these models for specific applications is beyond the scope of this paper and is left to their potential users.

II. Continuous-Time Markov Chain

A CTMC is a continuous-time stochastic process taking values in a discrete set isomorphic to $\{1, 2, \ldots, n\}$. As shown in Fig. 2, this stochastic process has piecewise constant sample paths with abrupt jumps at random times from some value in $\{1, 2, \ldots, n\}$ (called state) to another. This section explains how CTMCs can be used to describe the dynamics of interacting agents on an Ising lattice, of course, for a large value of n combinatorially increasing with the lattice size. Yet, the main goal of this section is to provide the technical background necessary for construction of lower complexity models introduced in Section III.

A. Master Equation and Continuous-Time Markov Chains

Suppose $\{x(t)\}$ is a CTMC taking values in the discrete set $\mathscr{X} = \{1, 2, \ldots, n\}$. Let $p(t) = [p_1(t) \;\; p_2(t) \cdots p_n(t)]^T$ be an $n \times 1$ vector containing the probabilities

$$p_k(t) = \Pr\{x(t) = k\}, \quad k = 1, 2, \ldots, n$$

of the CTMC being in the state k (i.e., taking the value k) at time t. Then, the temporal evolution of $p(t)$ is governed [16] by the linear dynamics

$$\dot{p}(t) = A(t)\, p(t), \tag{1}$$

where $A(t)$ is the $n \times n$ transition rate matrix of the CTMC. This matrix consists of nonnegative off-diagonal elements denoted by $a_{ij}(t) \geqslant 0$, $i \neq j$, and the diagonal elements

$$a_{ii}(t) = -\sum_{j=1,\, j\neq i}^{n} a_{ji}(t), \quad i = 1, 2, \ldots, n. \tag{2}$$

Here, $a_{ij}(t)$, $i \neq j$ represents the transition rate from state j to state i at time t.

Consider a system of K unlabeled, identical agents which interact on an Ising lattice with $L > K$ sites, accommodating at most one agent each. These K agents can be distributed among L sites of the lattice in

$$n = \frac{L!}{K!\,(L-K)!} \tag{3}$$

different ways, each regarded as an instance of the collective state of the agents. These instances are labeled by numbers 1 through n, and a probability $p_k(t)$ is assigned to the event that the instance $k = 1, 2, \ldots, n$ occurs at time t. Then, if the transition rate from instance j to instance $i \neq j$ at time t is known to be $a_{ij}(t)$, the temporal evolution of probabilities is governed by a master equation of the form (1).

As this equation identically governs the temporal evolution of probability distribution in a CTMC, the dynamics of a set of interacting agents on an Ising lattice can be represented by a CTMC. The disadvantage of this approach is the potentially gigantic size of the state space $\mathscr{X}$ of the CTMC, depending combinatorially on the size of Ising lattice according to (3). Section III of this paper introduces alternative models with substantially lower complexity. These models rely on some extension of the notion of CTMC discussed in the remainder of this section.

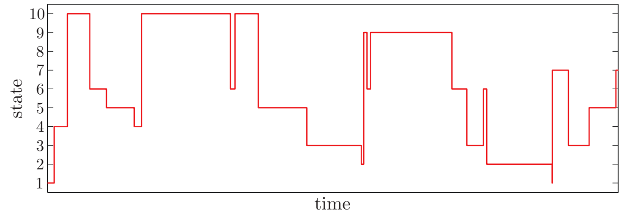

Fig. 2. Typical sample path of a CTMC with values in $\{1, 2, \ldots, 10\}$.

B. Representation by Stochastic Differential Equations

A CTMC can be constructed explicitly as the solution to a stochastic differential equation (SDE) studied in this section. This SDE constructs an n-state CTMC in terms of $n(n-1)$ statistically independent Poisson counters. Suppose $\{N_{ij}(t)\}$ is a nonhomogeneous Poisson counter with the intensity (or rate) $a_{ij}(t)$, and assume $\{N_{ij}(t)\}$, $i, j = 1, 2, \ldots, n$, $i \neq j$ are statistically independent. Let $\delta(\cdot)$ denote the Kronecker delta function defined as

$$\delta(z) = \begin{cases} 1 & z = 0 \\ 0 & z \neq 0 \end{cases}.$$

Then, the CTMC $\{x(t)\}$ can be represented for $t > 0$ as the solution to the SDE [16, p. 29]

$$dx(t) = \sum_{i=1}^{n} \sum_{\substack{j=1 \\ j\neq i}}^{n} (i-j)\, \delta(x(t)-j)\, dN_{ij}(t) \tag{4}$$

with a random initial state $x(0)$ drawn from some probability distribution defined on $\mathscr{X} = \{1, 2, \ldots, n\}$.

For sake of simplicity in the remainder of the paper, the set

$$\mathcal{S}_n = \{(i,j) \,|\, i, j = 1, 2, \ldots, n, \; i \neq j\}$$

is defined and the double summation in (4) is replaced by a single summation on $\mathcal{S}_n$ as a shorthand. Then, the SDE (4) is expressed in the compact form

$$dx(t) = \sum_{\mathcal{S}_n} (i-j)\,\delta(x(t)-j)\,dN_{ij}(t)\,.$$

This SDE is interpreted as follows by rewriting it in the integral form

$$x(t) = x(0) + \sum_{\mathcal{S}_n} (i-j) \int_0^t \delta(x(\tau)-j)\,dN_{ij}(\tau)\,.$$

Let τ_{m-1} and τ_m denote two successive transition times of the Poisson counter $\{N_{ij}(t)\}$. Then, the integral taken with respect to this Poisson counter on the right-hand side of this equation is defined in such a manner to remain constant over the interval $t \in (\tau_{m-1}, \tau_m]$, and to experience a discontinuity of the magnitude $\delta(x(\tau_m)-j)$ at the transition time τ_m.

The following proposition verifies that the solution $\{x(t)\}$ to the SDE (4) has a probability distribution evolving in time according to the master equation (1).

Proposition 1: The stochastic process $\{x(t)\}$ generated as the solution of the SDE (4) is a CTMC in the sense that its probability distribution $p(t)$ evolves in time according to (1).

Proof: For every $t \geqslant 0$, let $s = \omega\sqrt{-1}$ and define the characteristic function of the random variable $x(t)$ as

$$\phi(s,t) = \mathrm{E}\left[\exp(sx(t))\right]. \tag{5}$$

Since the characteristic function carries the same information as the probability distribution, it is enough to equivalently describe the temporal evolution of (5). To that end, fix s and apply the Itô differentiation rule of jump processes [16, p. 31] to $\exp(sx(t))$ in order to obtain

$$\begin{aligned} d\exp(sx(t)) &= \sum_{\mathcal{S}_n} \Big(\exp(sx(t) + s(i-j)\,\delta(x(t)-j)) \\ &\qquad - \exp(sx(t)) \Big) dN_{ij}(t) \\ &= \sum_{\mathcal{S}_n} \left(e^{is} - e^{js}\right) \delta(x(t)-j)\,dN_{ij}(t)\,, \end{aligned} \tag{6}$$

where the second equality is concluded from the identity

$$\begin{aligned} &\exp(sx(t) + s(i-j)\,\delta(x(t)-j)) \\ &\qquad = \exp(sx(t)) + \left(e^{is} - e^{js}\right) \delta(x(t)-j)\,. \end{aligned}$$

Taking the expected value of both sides of (6) leads to

$$\begin{aligned} d\phi(s,t) &= \mathrm{E}\left[\sum_{\mathcal{S}_n} \left(e^{is} - e^{js}\right) \delta(x(t)-j)\,dN_{ij}(t) \right] \\ &= \sum_{\mathcal{S}_n} \mathrm{E}\left[\left(e^{is} - e^{js}\right) \delta(x(t)-j) \right] \mathrm{E}\left[dN_{ij}(t)\right], \end{aligned} \tag{7}$$

where the second equality is concluded from the fact that the stochastic process $\{N_{ij}(t)\}$ has independent increments. By replacing $\mathrm{E}[dN_{ij}(t)]$ with $a_{ij}(t)\,dt$ and dividing both sides of (7) by dt, it is concluded that

$$\frac{\partial\phi(s,t)}{\partial t} = \sum_{\mathcal{S}_n} \left(e^{is} - e^{js}\right) a_{ij}(t)\,\mathrm{E}\left[\delta(x(t)-j)\right]. \tag{8}$$

Let $p_k(t)$, $k = 1, 2, \ldots, n$ denote $\Pr\{x(t) = k\}$. Then, it is straightforward to show $\mathrm{E}[\delta(x(t)-j)] = p_j(t)$ and

$$\frac{\partial\phi(s,t)}{\partial t} = \sum_{i=1}^{n} \dot{p}_i(t)\,e^{is}.$$

By substituting these expressions into (8) and then matching the coefficients of e^{is}, $i = 1, 2, \ldots, n$ in both sides of the resulting equation, a set of n linear equations is obtained as

$$\dot{p}_i(t) = -\sum_{j=1,\, j\neq i}^{n} a_{ji}(t)\,p_i(t) + \sum_{j=1,\, j\neq i}^{n} a_{ij}(t)\,p_j(t)$$

for $i = 1, 2, \ldots, n$. According to (2), the first summation on the right-hand side is equal to $a_{ii}(t)\,p_i(t)$, so these equations in a vector form are the same as the master equation (1). ■

C. Doubly Stochastic Continuous-Time Markov Chain

The CTMC constructed by the SDE (4) can conveniently describe the controlled dynamics of interacting agents under a deterministic control vector $u(t)$. This control vector can be included in the SDE (4) by simply taking the time-varying intensities $a_{ij}(t)$ of the Poisson counters $\{N_{ij}(t)\}$ explicit functions $a_{ij}(t) = a_{ij}(u(t))$ of the control vector $u(t)$. An extension of this procedure to a stochastic control is possible but not as straightforward as the deterministic case. Yet, such extension is necessary for a control generated by a feedback loop involving measurements of the CTMC itself, or even more crucial to this paper, in the case that the dynamics of a CTMC is impacted by the state of another CTMC.

For this latter scenario considered in Section III, the notion of CTMC is extended to the more general notion of doubly stochastic (conditional) CTMC. Roughly speaking, a doubly stochastic CTMC is a stochastic process that behaves similar to a CTMC, when conditioned on its stochastic transition rate matrix. Within the framework of this paper, construction of such stochastic process is straightforward by generalizing the notion of Poisson counter used in the SDE (4) to the notion of doubly stochastic Poisson counter (or Cox process), which is well studied in the theory of stochastic processes [17].

Suppose that $\{a(t)\}$ is a nonnegative stochastic process. Then, $\{N(t)\}$ is called a doubly stochastic Poisson counter, if conditioned on $\{a(t)\}$, it has the same statistical properties of a nonhomogeneous Poisson counter with the rate $a(t)$. For convenience of notation, a doubly stochastic Poisson counter with the rate $\{a(t)\}$ is denoted in this paper by $\{\mathcal{N}(a(t))\}$. In addition, it is assumed that $\{\mathcal{N}(a_i(t))\}$, $i = 1, 2, \ldots, \ell$ are independent, conditioned on $\{a_i(t)\}$, $i = 1, 2, \ldots, \ell$.

Using the notation of doubly stochastic Poisson counter, the SDE (4) can be modified into

$$dx(t) = \sum_{\mathcal{S}_n} (i-j)\,\delta(x(t)-j)\,d\mathcal{N}(a_{ij}(t)) \tag{9}$$

in order to construct a doubly stochastic CTMC $\{x(t)\}$ with the stochastic transition rates $\{a_{ij}(t)\}$, $(i,j) \in \mathcal{S}_n$. These transition rates can be explicit functions of some stochastic process that represent a control vector or the state of other doubly stochastic CTMCs. For the stochastic process $\{x(t)\}$ generated by the SDE (9), describing the temporal evolution of probability distribution requires an equation more complex than (1). The following proposition provides some insight into this issue.

Proposition 2: Let $\{x(t)\}$ be the solution to the SDE (9) with the stochastic transition rates $\{a_{ij}(t)\}$. Denote by $p_k(t)$ the probability of event $x(t)=k$ for $k=1,2,\dots,n$. Then, the probabilities $p_k(t)$ evolve in time according to the system of coupled linear differential equations

$$\dot{p}_i(t) = -\sum_{j=1,\, j\neq i}^{n} \hat{a}_{ji}(t)\, p_i(t) + \sum_{j=1,\, j\neq i}^{n} \hat{a}_{ij}(t)\, p_j(t) \tag{10}$$

for $i=1,2,\dots,n$. Here, $\hat{a}_{ij}(t)$ is a deterministic function defined via the conditional expectation

$$\hat{a}_{ij}(t) = \mathrm{E}\left[a_{ij}(t)\,|x(t)=j\right]. \tag{11}$$

Proof: The proof parallels the proof of Proposition 1 with minor modifications. The characteristic function of $x(t)$ is defined similar to (5), and then, it is shown that

$$\begin{aligned} d\phi(s,t) &= \sum_{\mathcal{S}_n} \mathrm{E}\Big[\mathrm{E}\big[\left(e^{is}-e^{js}\right)\delta\left(x(t)-j\right) \\ &\qquad\qquad \times dN_{ij}(t)\,|a_{ij}(t)\big]\Big] \\ &= \sum_{\mathcal{S}_n} \mathrm{E}\Big[\mathrm{E}\big[\left(e^{is}-e^{js}\right)\delta\left(x(t)-j\right)|a_{ij}(t)\big] \\ &\qquad\qquad \times \mathrm{E}\big[dN_{ij}(t)\,|a_{ij}(t)\big]\Big] \\ &= \sum_{\mathcal{S}_n} \left(e^{is}-e^{js}\right) \mathrm{E}\Big[a_{ij}(t)\,\delta\left(x(t)-j\right)\Big]dt. \end{aligned} \tag{12}$$

Here, the first equality represents the smoothing property of conditional expectation and the second is concluded from the fact that $\{N_{ij}(t)\}$ has conditionally independent increments. The last equality is obtained by replacing $\mathrm{E}\left[dN_{ij}(t)\,|a_{ij}(t)\right]$ with $a_{ij}(t)\,dt$ in the second equality and noting that the other conditional expectation is measurable with respect to $a_{ij}(t)$.

Dividing both sides of (12) by dt and then substituting

$$\mathrm{E}\left[a_{ij}(t)\,\delta\left(x(t)-j\right)\right] = \mathrm{E}\left[a_{ij}(t)\,|x(t)=j\right]p_j(t)$$

into the resulting equation yield

$$\frac{\partial\phi(s,t)}{\partial t} = \sum_{\mathcal{S}_n}\left(e^{is}-e^{js}\right)\hat{a}_{ij}(t)\,p_j(t).$$

By applying a coefficient matching procedure to this equation similar to (7), the differential equations (10) are obtained. ■

Remark 1: Although the differential equations (10) have an apparently simple structure resembling a master equation, they cannot be easily applied for computation of probability distribution in practice, since the coefficients $\hat{a}_{ij}(t)$ of these equations cannot be straightforwardly computed via (11).

III. Coupled Stochastic Differential Equations

Consider K unlabeled, identical agents living on an Ising lattice with $L>K$ sites, and dynamically change their states as a result of mutual interactions and possibly some external control. In Section II-A, the collective dynamics of the agents was modeled using a high dimensional master equation, or equivalently, a large CTMC. In this section, two new models are constructed with lower complexity based on the SDE (9) introduced in Section II-C.

A. Coupled SDEs Representing the Agents

In the first model, the state of each agent is expressed by a doubly stochastic CTMC which takes values in the discrete set $\{1,2,\dots,L\}$, including the labels of L sites of an Ising lattice. Each of the K doubly stochastic CTMC is generated by an SDE of the form (9) in which the stochastic transition rates are explicit functions of the state of other $K-1$ agents. Then, the collective dynamics of all K agents is represented by a set of K coupled SDEs described below.

Suppose that agent $k=1,2,\dots,K$ is represented by the doubly stochastic CTMC $\{x_k(t)\}$. Then, the collective state of the agents is represented by the vector

$$\mathbf{x}(t) = \begin{pmatrix} x_1(t) & x_2(t) & \cdots & x_K(t)\end{pmatrix}$$

in $\{1,2,\dots,L\}^K$. The complement of $x_k(t)$ is defined as a vector $\mathbf{x}_k^c(t)$ in $\{1,2,\dots,L\}^{K-1}$ constructed by removing the element $x_k(t)$ of $\mathbf{x}(t)$. The $L\times L$ stochastic transition rate matrix of $\{x_k(t)\}$ is a function of $\mathbf{x}_k^c(t)$, and possibly, a stochastic control vector $u(t)$ and time t. In the rest of this paper, only the dependence on $\mathbf{x}_k^c(t)$ is explicitly shown, for sake of simplicity, i.e., the transition rate matrix k is given by

$$A_k(t) = F\left(\mathbf{x}_k^c(t)\right).$$

Here, $F(\cdot)$ is a matrix-valued function of $K-1$ variables, and is invariant under any permutation of its variables, which reflects the assumption that the agents are unlabeled and identical. The elements of $F(\cdot)$ are denoted by $f_{ij}(\cdot)$. These elements hold the property that $f_{ij}(z_1,z_2,\dots,z_{K-1})=0$, if any of its arguments $z_1,z_2,\dots,z_{K-1}$ takes the value of i. This property disallows the agents reoccupying a lattice site already occupied by another agent.

Based on SDE (9) and using the notation introduced above, the dynamics of K interacting agents can be represented by a set of K coupled SDEs

$$dx_k(t) = \sum_{\mathcal{S}_L}(i-j)\,\delta\big(x_k(t)-j\big)d\mathcal{N}\big(f_{ij}\left(\mathbf{x}_k^c(t)\right)\big) \tag{13}$$

for $k=1,2,\dots,K$, or explicitly, in the vector form

$$\begin{aligned} dx_1(t) &= \sum_{\mathcal{S}_L}(i-j)\,\delta\big(x_1(t)-j\big)d\mathcal{N}\big(f_{ij}\left(\mathbf{x}_1^c(t)\right)\big) \\ dx_2(t) &= \sum_{\mathcal{S}_L}(i-j)\,\delta\big(x_2(t)-j\big)d\mathcal{N}\big(f_{ij}\left(\mathbf{x}_2^c(t)\right)\big) \\ &\vdots \\ dx_K(t) &= \sum_{\mathcal{S}_L}(i-j)\,\delta\big(x_K(t)-j\big)d\mathcal{N}\big(f_{ij}\left(\mathbf{x}_K^c(t)\right)\big). \end{aligned}$$

Here, the coupling between the SDEs is established via the complement vectors $\mathbf{x}_1^c(t), \mathbf{x}_2^c(t), \dots, \mathbf{x}_K^c(t)$ involved in the transition rates on the right-hand side. The random initial state $\mathbf{x}(0)$ of the coupled SDEs is drawn from a probability distribution defined on $\{1,2,\dots,L\}^K$, with zero probability assigned to the events in which more than one agents occupy a single lattice site.

To implement the set of SDEs (13), a total of $KL(L-1)$ doubly stochastic Poisson counters are needed that is roughly proportional to the square of the number of lattice sites. This number shows a far lower complexity than $n(n-1)$ for a master equation model in which n depends combinatorially on L according to (3). As an illustrative example, for $K=50$ and $L=400$, these figures are 2.9×10^{128} versus 8×10^{6}, respectively for a master equation model and for the coupled SDEs (13). Of course, such drastic reduction in complexity comes at a price: the SDE model in (13) is not as flexible as the master equation model. This issue is discussed next based on the following proposition which describes the temporal evolution of probability distribution in the set of SDEs (13).

Proposition 3: Let $\mathbf{x}(t)\in\{1,2,\ldots,L\}^K$ be the solution to the set of coupled SDEs (13) and define its characteristic function as

$$\phi(\mathbf{s},t)=\mathrm{E}\left[\exp\left(\mathbf{s}\cdot\mathbf{x}(t)\right)\right],$$

where $\cdot$ denotes the dot product operator and $\mathbf{s}$ is given by

$$\mathbf{s}=\sqrt{-1}\begin{pmatrix}\omega_1 & \omega_2 & \cdots & \omega_K\end{pmatrix}. \tag{14}$$

Then, the temporal evolution of this function is governed by

$$\frac{\partial\phi(\mathbf{s},t)}{\partial t}=\sum_{k=1}^{K}\sum_{\mathcal{S}_L}\left(e^{is_k}-e^{js_k}\right)\mathrm{E}\Big[f_{ij}\left(\mathbf{x}_k^c(t)\right) \times\exp\left(\mathbf{s}_k^c\cdot\mathbf{x}_k^c(t)\right)\delta\big(x_k(t)-j\big)\Big], \tag{15}$$

where s_k is the element k of $\mathbf{s}$ defined by (14), and $\mathbf{s}_k^c$ is a vector in $\mathbb{C}^{K-1}$ constructed by removing element s_k from $\mathbf{s}$.

Proof: Using the product rule of differentiation first and then applying the Itô differentiation rule similar to (6) lead to

$$\begin{aligned} d\phi(\mathbf{s},t)&=\mathrm{E}\left[d\exp\left(\mathbf{s}\cdot\mathbf{x}(t)\right)\right]\\ &=\mathrm{E}\left[\sum_{k=1}^{K}\exp\left(\mathbf{s}_k^c\cdot\mathbf{x}_k^c(t)\right)d\exp\big(s_kx_k(t)\big)\right]\\ &=\mathrm{E}\Bigg[\sum_{k=1}^{K}\exp\left(\mathbf{s}_k^c\cdot\mathbf{x}_k^c(t)\right)\sum_{\mathcal{S}_L}\left(e^{is_k}-e^{js_k}\right)\\ &\qquad\times\delta\big(x_k(t)-j\big)d\mathcal{N}\big(f_{ij}\left(\mathbf{x}_k^c(t)\right)\big)\Bigg]. \end{aligned}$$

Then, a procedure parallel to (12) yields (15). ∎

Using an extension of the coefficient matching technique in Proposition 1, a set of linear differential equations can be derived from (15) to characterize the temporal evolution of probability distribution in the system of coupled SDEs (13). Specifically, let $\mathbf{i}$ be a vector in the discrete set

$$\mathbb{I}=\left\{(i_1,i_2,\ldots,i_K)\,|\,i_1\neq i_2\neq\cdots\neq i_K\in\{1,2,\ldots,L\}\right\}$$

containing the instances of the stochastic vector $\mathbf{x}(t)$ solving the coupled SDEs (13). Define the set of probabilities

$$p_{\mathbf{i}}(t)=\Pr\left\{\mathbf{x}(t)=\mathbf{i}\right\},\quad \mathbf{i}\in\mathbb{I}.$$

For each $\mathbf{i}\in\mathbb{I}$, the probability $p_{\mathbf{i}}(t)$ is corresponding to the probability $p_k(t)$ assigned to some instance k of a CTMC with a large state space $\mathscr{X}=\{1,2,\ldots,n\}$ for n given by (3).

By matching the coefficients of $e^{\mathbf{i}\cdot\mathbf{s}}$ in (15) for $\mathbf{i}\in\mathbb{I}$, a set of n linear differential equations is obtained with $\dot{p}_{\mathbf{i}}(t)$ on their left-hand sides and a linear combination of $p_{\mathbf{j}}(t)$, $\mathbf{j}\in\mathbb{I}$ on their right-hand sides, where the coefficients of each linear combination is determined in terms of the functions $f_{ij}(\cdot)$. This set of linear differential equations introduces a master equation of the form (1), which in turn, is corresponding to a CTMC. Hence, the stochastic process $\{\mathbf{x}(t)\}$ generated by the coupled SDEs (13) is equivalent to a CTMC with a large state space $\mathscr{X}=\{1,2,\ldots,n\}$.

However, the transition rate matrix of this CTMC is not arbitrarily chosen, instead, it is determined in terms of the functions $f_{ij}(\cdot)$ in (13) within certain constrained structure. In addition, this matrix is sparse by the following argument. The probability of simultaneous transitions in two or more conditionally independent Poisson counters is 0, thus in each transition time only a single element of the vector $\mathbf{x}(t)$ can change. This simply implies that the transition rates between two instances $\mathbf{i},\mathbf{j}\in\mathbb{I}$ of $\mathbf{x}(t)$ with $\|\mathbf{i}-\mathbf{j}\|_0>1$ must be identically 0. Here, the 0-norm $\|\cdot\|_0$ counts the number of nonzero elements of a vector.

B. Coupled SDEs Representing the Lattice Sites

In this section, the state of a system of K agents living in an Ising lattice with L sites is represented by a vector of L binary elements such that at any time t, exactly K elements of this vector take the value 1 and the remaining take 0. Each element of this vector is assigned to a lattice site, signifying the presence or absence of an agent in that site. This binary vector is then modeled as a stochastic process generated by a set of L coupled SDEs representing its L elements.

Denote the vector of binary stochastic processes by

$$\mathbf{y}(t)=\begin{pmatrix}y_1(t) & y_2(t) & \cdots & y_L(t)\end{pmatrix}.$$

The transition rate from the lattice site j to another site i is a nonnegative stochastic process given by a function $\lambda_{ij}(\mathbf{y}(t))$ of the state $\mathbf{y}(t)$ of all L sites. More generally, this rate can be a function of a stochastic control vector $u(t)$ and time t according to $\lambda_{ij}(\mathbf{y}(t),u(t),t)$. For sake of simplicity, the possible dependence of the transition rates on control and time is not explicitly shown in this paper.

Using the concept of doubly stochastic Poisson counter, the temporal evolution of the stochastic vector $\mathbf{y}(t)$ can be represented by a system of L coupled SDEs

$$\begin{aligned} dy_i(t)=&-\sum_{j=1,\ j\neq i}^{L}y_i(t)\big(1-y_j(t)\big)d\mathcal{N}\big(\lambda_{ji}(\mathbf{y}(t))\big)\\ &+\sum_{j=1,\ j\neq i}^{L}\big(1-y_i(t)\big)y_j(t)\,d\mathcal{N}\big(\lambda_{ij}(\mathbf{y}(t))\big) \end{aligned} \tag{16}$$

for $i=1,2,\ldots,L$. These equations are constructed in such a manner that a transition of an element $y_k(t)$ from $0/1$ to $1/0$ is concurrent with the transition from $1/0$ to $0/1$ of another element $y_{k'}(t)$, and as a consequence, the number of elements with the value 1 remains unchanged over time. The initial state $\mathbf{y}(0)$ of the set of equations (16) is drawn from a probability distribution on $\{0,1\}^L$ satisfying

$$\Pr\left\{\|\mathbf{y}(0)\|_1=K\right\}=1,$$

where $\|\cdot\|_1$ denotes norm 1 of vectors. Then, it holds that

$$\Pr\{\|\mathbf{y}(t)\|_1 = K\} = 1, \quad t \geqslant 0.$$

The system of coupled SDEs (16) can be constructed using only $L(L-1)$ doubly stochastic Poisson counters, far less than $n(n-1)$ Poisson counters needed for a CTMC model, and less than $KL(L-1)$ doubly stochastic Poisson counters required for the coupled SDEs (13). An analysis similar to Section III-A applied to Proposition 4 below, indicates that the solution $\{\mathbf{y}(t)\}$ to the coupled SDEs (16) is equivalent to a CTMC of large combinatorial dimension n in (3). Yet, this CTMC has a sparse transition rate matrix constrained within some predetermined structure, consisted of the transition rate functions $\lambda_{ij}(\cdot)$ in (16).

Proposition 4: Assume that $\mathbf{y}(t) \in \{0,1\}^L$ is the solution to the set of coupled SDEs (16) and define its characteristic function as

$$\phi(\mathbf{s}, t) = \mathrm{E}\left[\exp(\mathbf{s} \cdot \mathbf{y}(t))\right],$$

where $\cdot$ denotes the dot product operator and $\mathbf{s}$ is given by

$$\mathbf{s} = \sqrt{-1}\begin{pmatrix}\omega_1 & \omega_2 & \cdots & \omega_L\end{pmatrix}. \tag{17}$$

Then, the temporal evolution of this function is governed by

$$\begin{aligned}\frac{\partial\phi(\mathbf{s},t)}{\partial t} = &-\sum_{\mathcal{S}_L}\left(1-e^{-s_i}\right)\mathrm{E}\Big[\exp(\mathbf{s}\cdot\mathbf{y}(t)) \\ &\qquad\times y_i(t)\left(1-y_j(t)\right)\lambda_{ji}(\mathbf{y}(t))\Big] \\ &+\sum_{\mathcal{S}_L}\left(e^{s_i}-1\right)\mathrm{E}\Big[\exp(\mathbf{s}\cdot\mathbf{y}(t)) \\ &\qquad\times\left(1-y_i(t)\right)y_j(t)\,\lambda_{ij}(\mathbf{y}(t))\Big],\end{aligned} \tag{18}$$

where s_i denotes element i of the vector $\mathbf{s}$ in (17).

Proof: Application of the Itô differentiation rule for jump processes [16, p. 31] to $\exp(s_i y_i(t))$ results in

$$\begin{aligned}d\exp\big(s_i y_i(t)\big) &= \sum_{j=1,\, j\neq i}^{L}\Big(\exp\big(s_i y_i(t) - s_i y_i(t)(1-y_j(t))\big) \\ &\qquad - \exp\big(s_i y_i(t)\big)\Big)d\mathcal{N}\big(\lambda_{ji}(\mathbf{y}(t))\big) \\ &\quad+\sum_{j=1,\, j\neq i}^{L}\Big(\exp\big(s_i y_i(t) + s_i(1-y_i(t))\,y_j(t)\big) \\ &\qquad - \exp\big(s_i y_i(t)\big)\Big)d\mathcal{N}\big(\lambda_{ij}(\mathbf{y}(t))\big) \\ &= -\sum_{j=1,\, j\neq i}^{L}\left(e^{s_i}-1\right)y_i(t)\left(1-y_j(t)\right)d\mathcal{N}\big(\lambda_{ji}(\mathbf{y}(t))\big) \\ &\quad+\sum_{j=1,\, j\neq i}^{L}\left(e^{s_i}-1\right)\left(1-y_i(t)\right)y_j(t)\,d\mathcal{N}\big(\lambda_{ij}(\mathbf{y}(t))\big).\end{aligned}$$

This expression is substituted into

$$\begin{aligned}d\phi(\mathbf{s},t) &= \mathrm{E}\left[d\exp(\mathbf{s}\cdot\mathbf{y}(t))\right] \\ &= \mathrm{E}\left[\sum_{i=1}^{L}\exp\left(\mathbf{s}\cdot\mathbf{y}(t) - s_i y_i(t)\right)d\exp\left(s_i y_i(t)\right)\right]\end{aligned}$$

which is concluded from the product rule of differentiation. The resulting equation is then converted to (18) by following a procedure similar to (12). ■

IV. Conclusion

Two stochastic models were proposed to characterize the dynamics of a system of multiple agents living on an Ising lattice and changing their discrete state at random times due to their internal interactions and possibly an external control. The models were constructed as systems of interacting SDEs driven by independent doubly stochastic Poisson counters, with a complexity growing polynomially with the lattice size. These SDEs were developed as low complexity alternatives to the more conventional models relying on high dimensional master equations (or equivalently CTMCs) with complexities growing combinatorially with the lattice size.

References

[1] N. L. Rosi and C. A. Mirkin, "Nanostructures in biodiagnostics," *Chemical Reviews*, vol. 105, no. 4, pp. 1547–1562, 2005.

[2] N. Stephanopoulos, E. O. Solis, and G. Stephanopoulos, "Nanoscale process systems engineering: Toward molecular factories, synthetic cells, and adaptive devices," *AIChE Journal*, vol. 51, no. 7, pp. 1858–1869, 2005.

[3] A. Winkleman, B. D. Gates, L. S. McCarty, and G. M. Whitesides, "Directed self-assembly of spherical particles on patterned electrodes by an applied electric field," *Advanced Materials*, vol. 17, no. 12, pp. 1507–1511, 2005.

[4] M. P. Stoykovich, H. Kang, K. C. Daoulas, G. Liu, C.-C. Liu, J. J. de Pablo, M. Müller, and P. F. Nealey, "Directed self-assembly of block copolymers for nanolithography: Fabrication of isolated features and essential integrated circuit geometries," *ACS Nano*, vol. 1, no. 3, pp. 168–175, 2007.

[5] R. A. Kiehl, "DNA-directed assembly of nanocomponents for nano-electronics, nanophotonics, and nanosensing," in *Proceddings of SPIE*, vol. 6768, pp. 67680Z–1–67680Z–7, 2007.

[6] M. Grzelczak, J. Vermant, E. M. Furst, and L. M. Liz-Marzán, "Directed self-assembly of nanoparticles," *ACS Nano*, vol. 4, no. 7, pp. 3591–3605, 2010.

[7] A. Komaee and P. I. Barton, "Potential canals for control of nonlinear stochastic systems in the absence of state measurements," *IEEE Transactions on Control Systems Technology*, vol. 25, no. 1, pp. 161–174, 2017.

[8] Y. Gao, B. W. Nyande, and R. Lakerveld, "Open-loop control of directed self-assembly of colloidal particles in a microfluidic device," *Computers & Chemical Engineering*, vol. 139, p. 106837, 2020.

[9] B. A. Cipra, "An introduction to the Ising model," *The American Mathematical Monthly*, vol. 94, no. 10, pp. 937–959, 1987.

[10] E. O. Solis, P. I. Barton, and G. Stephanopoulos, "Controlled formation of nanostructures with desired geometries. 1. robust static structures," *Industrial & Engineering Chemistry Research*, vol. 49, no. 17, pp. 7728–7745, 2010.

[11] E. O. Solis, P. I. Barton, and G. Stephanopoulos, "Controlled formation of nanostructures with desired geometries. 2. robust dynamic paths," *Industrial & Engineering Chemistry Research*, vol. 49, no. 17, pp. 7746–7757, 2010.

[12] R. Lakerveld, G. Stephanopoulos, and P. I. Barton, "A master-equation approach to simulate kinetic traps during directed self-assembly," *The Journal of Chemical Physics*, vol. 136, no. 18, p. 184109, 2012.

[13] S. Ramaswamy, R. Lakerveld, P. I. Barton, and G. Stephanopoulos, "Controlled formation of nanostructures with desired geometries: Part 3. dynamic modeling and simulation of directed self-assembly of nanoparticles through adaptive finite state projection," *Industrial & Engineering Chemistry Research*, vol. 54, no. 16, pp. 4371–4384, 2015.

[14] A. Komaee and P. I. Barton, "Directed self-assembly of linear nanostructures by optimal control of external electrical fields." arXiv preprint arXiv:1603.00113, 2016.

[15] B. Munsky and M. Khammash, "The finite state projection algorithm for the solution of the chemical master equation," *The Journal of Chemical Physics*, vol. 124, no. 4, p. 044104, 2006.

[16] R. Brockett, *Stochastic Control*. Lecture Notes, Harvard University, 2009.

[17] D. L. Snyder, *Random Point Processes*. Wiley-Interscience, 1975.