Complex Systems **2** (1988) 259–267

Simple Lattice Gas Models for Waves

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Abstract. A simple lattice gas model for solving the linear wave equation is presented. In this model a photon representation is used. Energy and momentum are shown to be conserved.

1. Introduction

The rapidly developing cellular automata (CA) theory, known also as the lattice gas method, has recently generated wide interest for modeling many different physical processes described generally by partial differential equations [1–5]. A lattice gas system consists of "particles" moving on a lattice satisfying certain symmetry requirements. The updating of the system is realized by designing microscopic rules for the moving and scattering of the particles. The solution of the partial differential equation of interest is usually approximated in terms of the averaged behavior of a set of microscopic quantities.

We can list three significant aspects of using the lattice gas method to study physical systems. First, since all particle interactions are local, this method provides a way to utilize concurrent architectures [6]. The advent of computers with 10^6 to 10^9 processors would allow computations to be done at 10^4 to 10^7 times present speeds with slower and therefore more reliable processors. Consequently, it is expected that the CA techniques will become a very important computational tool for numerical modeling. Second, because the CA operates with only integers and Boolean algebra, it requires less computer storage so that the spatial and time resolution can be much higher than other methods. For example 8×10^9 particles can be followed on existing Cray Solid State Disks containing 512 megawords. Many realistic physical processes can be simulated more accurately without roundoff or instabilities. Third, this method may provide new insight in understanding the relationship between the microscopic machanisms and the macroscopic behavior for some many-body physical systems.

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The CA theory has been successful in modeling fluids [1,2,4], magnetofluids [3,5] and other systems [7]. It also appears in principle that most physical systems with diffusive macroscopic dynamics can be approximated by CA models. The macroscopic behavior of some diffusive systems can be described by the following parabolic equation:

$$\frac{\partial f(\mathbf{x},t)}{\partial t} = F(t,\mathbf{x};f) + D\nabla^2 f(\mathbf{x},t), \tag{1.1}$$

where the macroscopic quantity $f(\mathbf{x},t)$ represents, for example, the averaged lattice particle density. The parameter D is the diffusivity. $F(t,\mathbf{x};f)$ is usually a nonlinear function of f.

It is of equal importance to investigate whether or not physical processes described by the hyperbolic differential equations can be modeled within CA framework [8]. An important process of this kind is wave propagation. Wave propagation possesses several features which differ from the diffusion process. In this report, we present a simple CA model which simulates wave propagation and conserves energy and momentum.

2. The wave equation model

Wave propagation processes are described by many different types of equations. However, the basic mechanics contains a common feature which is described by the simplest linear wave propagation process governed by the following linear hypobolic equation:

$$\frac{\partial^2 u(\mathbf{x},t)}{\partial t^2} = C^2\nabla^2 u(\mathbf{x},t), \tag{2.1}$$

where u is the wave amplitude and C is the wave speed. A typical example is electrodynamics described by the Maxwell equations. Written in terms of the scalar potential ϕ and the vector potential $\mathbf{A}$ and using the Lorentz gauge, the Maxwell equations without sources can be written as two linear wave equations in the form of equation (2.1) for ϕ and $\mathbf{A}$, plus the continuity equation

$$\frac{\partial \phi}{\partial t} + \nabla \cdot \mathbf{A} = 0.$$

Comparing equation (2.1) with equation (1.1), one can see that the wave equation has a second order time derivative, while the diffusion equation has a first order time derivative. This is the major difference between a wave propagation and diffusion.

Two physical quantities are conserved in a linear wave propagation process: (a) the total wave energy, H, defined as:

$$H = \int d\mathbf{x}\{(\frac{\partial u}{\partial t})^2 + C^2(\nabla u)^2\}, \tag{2.2}$$

and (b) the total wave momentum $\mathbf{P}$:

$$\mathbf{P} = 2 \int d\mathbf{x}\{(\frac{\partial u}{\partial t})\nabla u - u\nabla(\frac{\partial u}{\partial t})\}. \tag{2.3}$$

It is important that both of these conservation laws are satisfied in any CA model for the wave equation.

The lattice gas model that we are presenting for the linear wave propagation process consists of a number of "photons" propagating on a lattice. The lattice is invariant under rotations with angles of $2\pi/B$. (For the two-dimensional square and triangular lattices, B equals 4 and 6, respectively. While for the one-dimensional lattice, B is equal to 2.) The distance between any two nearest neighbor sites of the lattice is c. A photon at a site of the lattice moves at each time step to one of its B nearest neighbors with speed c, if we set the time step equal to one time unit. Although we could in general let photons have many different speeds or even perform a random walk [4,5], only one speed is required for the linear wave.

We define two kinds of photons distinguished by a "spin" quantum number σ. One kind of photon has the values $\sigma = \xi$ and another has $-\xi$, respectively. They could be considered as particles and anti-particles. Moreover, we define a cancellation process: at a given position when there is a ξ photon and a $-\xi$ photon, a cancellation occurs so that both of these photons are destroyed. Therefore, after each cancellation only one kind photon is left, namely the kind originally having the larger number of photons. This macroscopic rule causes the total photon number to fluctuate. We let the total σ at a point in space represent the wave amplitude. The two different kinds of photons have the same magnitude but they differ in sign. The wave amplitude at a given location and time is defined to be the sum of the local σ. That is, if we define $N_a^\sigma(\mathbf{x}, t)$; $(\sigma = \xi, -\xi; a = 1, \ldots, B)$ to be the number of photons with quantum σ at a particular site $\mathbf{x}$ and time t moving with velocity $\hat{c}_a$ $(|\hat{c}_a| = c)$ in the direction a, then the microscopic wave amplitude is defined by

$$U(\mathbf{x}, t) = \sum_{a,\sigma} \sigma N_a^\sigma(\mathbf{x}, t).$$

For computational convenience, we further require that there are no more than N_0 photons with the same σ at any site of $\mathbf{x}$. This requirement causes the photons to behave somewhat like Fermi particles instead of Bosons. Only when N_0 is infinity do these CA photons become bosons. However, if we require $N_0 \gg$ (the total number of photons of either kind at any time), then these photons can be approximately considered as Bosons.

In order to formulate a wave model, the microscopic updating rules must be chosen. According to Huygen's principle, any spatial point on a wave front can be thought of as a new wave source. Hence, we consider at each site of the lattice there is a wave source which emits photons as isotropically as possible. The intensity of a source is defined as $\tilde{U}(\mathbf{x}, t)$. The number of photons emitted at time t from a source in direction $\mathbf{c}_a$ is equal to $m_a \times |\tilde{U}(\mathbf{x}, t)|$ $(m_a \geq 0; a = 1, \ldots, B)$. Using the wave amplitude definition above, we have

$$\sum_a m_a \tilde{U}(\mathbf{x}, t) = U(\mathbf{x}, t).$$

The integer m_a is dependent not only on the velocity state $\hat{c}_a$ but also, in general, on $\mathbf{x}$ and t. Only one type of photon, each with the same value of σ, is emitted from a lattice site. All photons emitted have the same sign as their source $\tilde{U}(\mathbf{x}, t)$. Hence, $\sigma\tilde{U} \geq 0$. After emitting photons, the source decays obeying the following relationship

$$\tilde{U}(\mathbf{x}, t+1) - \tilde{U}(\mathbf{x}, t) = -G(\mathbf{x}, t+1),$$

where G is the decay rate of the source $\tilde{U}$. The change of the decay rate follows the relation

$$G(\mathbf{x}, t+1) - G(\mathbf{x}, t) = \sum_{a,\sigma} \sigma\{N_a^\sigma(\mathbf{x}, t) - N_a^\sigma(\mathbf{x} + \hat{c}_a, t)\}$$

which is equal to the difference between the net photon σ emitted and the net photon σ absorbed at time t. It is straightforward to see that the combination of the above two microscopic updating rules leads to a second order time derivative for the evolution of the averaged source $\tilde{U}$ in the continuous limit. As soon as the relationship between the photon number N_a^σ and the wave source $\tilde{U}$ is determined by fixing the factor m_a, the evolution of the wave process will be completely determined. With different choices of m_a we are able to formulate different wave processes. In general, m_a can be chosen to be a function of U. However, the given wave equation becomes the linear wave equation (2.1) when the integer $m_a; (a = 1, \ldots, B)$ is a constant everywhere.

The boundary conditions for the wave CA systems are easy to implement. For example, the "fixed" boundary condition ($U(\mathbf{x}_0) = 0$) is realized by reversing the normal component (with respect to the boundary) of the velocity direction of the photons at the boundary while keeping the parallel component unchanged. The photon σ on the boundary is changed into $-\sigma$. Similarly, the "free" boundary condition ($\nabla_\perp U(\mathbf{x}_0) = 0$) can be realized by leaving the photon spin value σ unchanged.

The choice of the microscopic rules for formulating a linear wave process is not unique. Thus a criterion for chosing the best process is desired. Using Huygen's principle, we wish to require the photon sources to be as isotropic as possible. We call this requirement the isotropic condition. This condition implies that we need to put $m_a B = m$, $(a = 1, \ldots, B)$. Furthermore, it should be emphasized that since we use photons as the only information carriers from one place to another, any physical information cannot have a transport speed greater than the photon speed. If we define the effective photon speed in a given direction to be the distance between two neighboring sites along this direction divided by the minimum number of time steps require for a photon to go from one site another, then it can be seen that this speed depends on direction. The effective photon speed depends on the discrete velocity directions on a discrete lattice. A photon cannot always travel in a straight line in an arbitrary direction, hence there is a minimum effective photon speed c/ν ($\leq c$) for each model. For example,

under the isotropic condition, ν is equal to unity for one-dimensional lattice. $\nu = \sqrt{2}$ for two-dimensional square lattice associated with the diagonal direction of a two-dimensional square lattice. Likewise, we have $\nu = \sqrt{3}$ for three-dimensional square lattice. As a result, any physically meaningful wave propagation process should not have its wave speed C exceed c/ν. This sets an upper bound on allowed speeds for any information transfer. This condition can be violated if a wrong set of microscopic rules are selected. For instance, if the photon source intensity is too high and its emitted photons cannot attain enough speed to propagate away, cumulation will occur which in turn leads to instability. We refer to this requirement as the minimum speed condition, or the CA Courant condition. If both the isotropic condition and the minimum speed condition are satisfied, the evolution of the system obeys the following equation:

$$U(\mathbf{x},t+1)-2U(\mathbf{x},t)+U(\mathbf{x},t-1) = m\{\frac{1}{B}\sum_a U(\mathbf{x}+\hat{c}_a,t)-U(\mathbf{x},t)\} \quad (2.4)$$

Equation (2.4) defines a deterministic microscopic CA wave process with discrete space and time. It happens to have the same form as a finite difference equation. However, unlike the usual finite difference approximation, it contains no roundoff error and no numerical instability. With a particular choice of m the CA system conserves the microscopic energy and momentum. Moreover, in the limit that the lattice cell size is small compared with characteristic lengths and the time step size is small compared with characteristic times, the continuous linear wave equation (2.1) is recovered after making an ensemble averaging ($\langle U(\mathbf{x},t)\rangle = u(\mathbf{x},t)$) and a Taylor expansion in time and space.

We have proved that the wave model conserves the following two global quantities, if the microscopic wave equation (2.4), expressed in terms of integers, can be exactly satisfied:

$$H = \sum_{\mathbf{x}}[U(\mathbf{x},t)^2 - U(\mathbf{x},t+1) * U(\mathbf{x},t-1)]$$

and

$$\begin{aligned}\mathbf{P} &= \\ &\tfrac{1}{c^2}\ \sum_{\mathbf{x}}\sum_a \hat{c}_a\{U(\mathbf{x},t+1) * U(\mathbf{x}+\mathbf{c}_a,t) + U(\mathbf{x},t-1) * U(\mathbf{x}-\hat{c}_a,t) \\ &-\ U(\mathbf{x},t) * [U(\mathbf{x}+\hat{c}_a,t+1) + U(\mathbf{x}-\hat{c}_a,t-1)]\}.\end{aligned}$$

It can be shown that above H and $\mathbf{P}$ reduce to the usual H and $\mathbf{P}$ for the linear wave in the continuous space and time limit, as expressed in equations (2.2) and (2.3). Therefore these correspond to the microscopic energy and momentum for the CA wave system. The conservation of above two global quantities is equivalent to $H(t) = H(t+1)$ and $\mathbf{P}(t) = \mathbf{P}(t+1)$. That is, it can be shown that H and $\mathbf{P}$ expressed in terms of the quantities at time t are unchanged when we replace all the quantities by those at time $t+1$, using the microscopic wave equation (2.4).

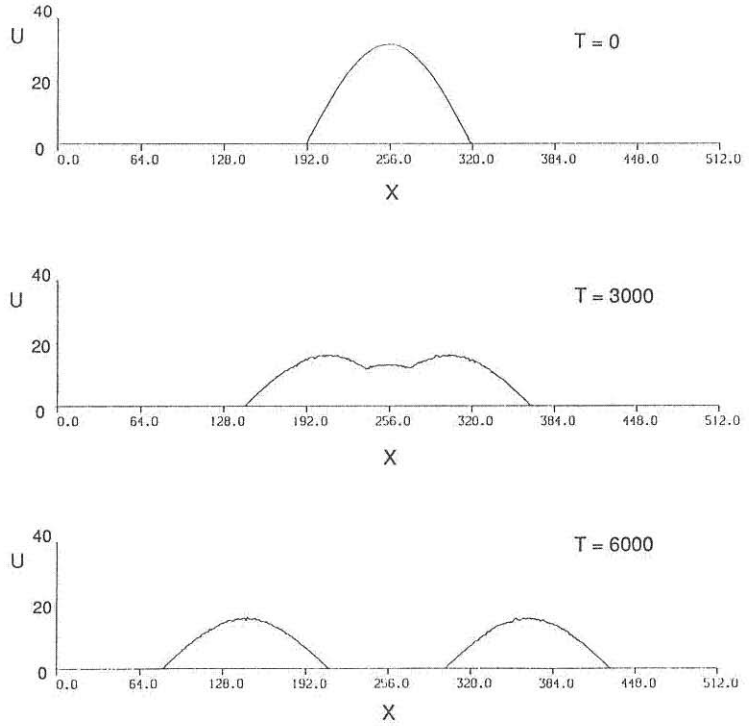

Figure 1: Evolution of a one-dimensional lattice gas wave at different time steps.

With the consideration of the CA Courant condition inequality, however, we have found that the microscopic energy H is a positive-definite quantity only when $B/m = \nu^2$ in equation (2.4). That is, the wave speed C must equal c/ν, the effective minimum photon speed. This leads to the conclusion that only the one-dimensional wave lattice gas model can satisfy the microscopic wave equation (2.4), since $\nu = 1$ in this case. Thus, it satisfies the microscopic conservation laws exactly. In higher dimensions the above global quantities H and $\mathbf{P}$ are conserved statistically. That is, we replace the microscopic wave amplitude U by its ensemble averaged value u $(= \langle U \rangle)$.

Results of a one-dimensional CA wave computer simulation are shown in figure 1 which describes the time evolution of a wave packet. This model is an exact microscopic wave process. The wave amplitude at $t < 0$ is set to be zero everywhere, while at $t = 0$ the amplitude is shown in the figure. As expected, the single wave packet evolves into a right-traveling wave packet and a left-traveling wave packet. Their shapes are preserved at all times.

For higher dimensional lattices the conservation laws are not exactly satisfied since $\nu > 1$, hence $m\tilde{U}(\mathbf{x}, t)$ may not always be evenly divided by B. It is in general impossible for the total number of photons emitted ($= m\tilde{U}(\mathbf{x}, t)$) to be distributed equally among all the B possible directions. In other words, $m_a; (a = 1, \ldots, B)$ can not be made exactly equal to m/B. Therefore equation (2.4) becomes only a statistical description of the wave CA for dimensions higher than 1.

Based on numerical experience, it is desirable, that both the isotropic condition and the CA Courant condition be satisfied as closely as possible in order to minimize microscopic fluctuations. One way to realize such a requirement in two-dimensional and three-dimensional, is first to distribute the total $m\tilde{U}(\mathbf{x}, t)$ ($m = 2$) photons equally among all the B directions, then put the possible remaining two photons into two anti-parallel directions. These two directions are selected with equal probability among all $B/2$ pairs of directions. In this way, it can be shown that the microscopic equation of motion of the CA wave system is

$$U(\mathbf{x}, t+1) - 2U(\mathbf{x}, t) + U(\mathbf{x}, t-1) = \sum_a m_a U(\mathbf{x} + \hat{c}_a, t) - mU(\mathbf{x}, t)$$

where $\sum_a m_a = m$ and the ensemble averaged $\langle m_a \rangle = m/B$, $(a = 1, \ldots, B)$. Thus equation (2.4) becomes statistically valid and the two above conservation laws are satisfied if we replace U by its averaged value.

As a result, we can use the wave CA model to simulate light experiments. For example, figure 2 gives the results of the two-dimensional wave CA simulation for the double-slit experiment at a given instant. In this simulation, 256×256 lattice cells are used. At 64 cells away from the left boundary a wall with two holes each with width of 5 cells is inserted, so that photons can go through the holes in order to go from left region into the right region. Elsewhere on the wall, photons will be reflected back. Initially, we put a plane sine-wave with amplitude of 16 $|\sigma|$ and wave length of 32 cells in the left region. The right region is empty initially. A spatial averaging is used with the average super-cell size of 4×4. As expected the wave amplitude exhibits a spatial interference pattern.

It is easy to see that the microscopic fluctuations δU ($\equiv U - \langle U \rangle$) induced by the above method in two-dimensional and three-dimensional also approximately follow equation (2.4) except that an additional white noise source with maximum magnitude of $|\sigma|$ appears. Using standard mathematics it can be shown that the root mean square value of the fluctuation of a individual Fourier mode at large time t is

$$\sqrt{\langle (\delta U(\mathbf{k}, t))^2 \rangle} = |\sigma / \mathrm{k}| \sqrt{t},$$

where the wave number $\mathbf{k}$ satisfies $2\pi/c \geq |\mathrm{k}| \geq 2\pi/L$, and L is the system size. This indicates that the maximum spatial *rms* fluctuation $\sqrt{\langle (\delta U)^2 \rangle}$ is approximately $|\sigma|\sqrt{t}$, and the maximum spatial correlation of the fluctuation $\langle \delta U(\mathbf{x}) \delta U(\mathbf{x} + \mathbf{r}) \rangle$ $(c \leq |\mathbf{r}| \leq L)$ is about $\sigma^2 ct/|\mathbf{r}|$ for three-dimensional

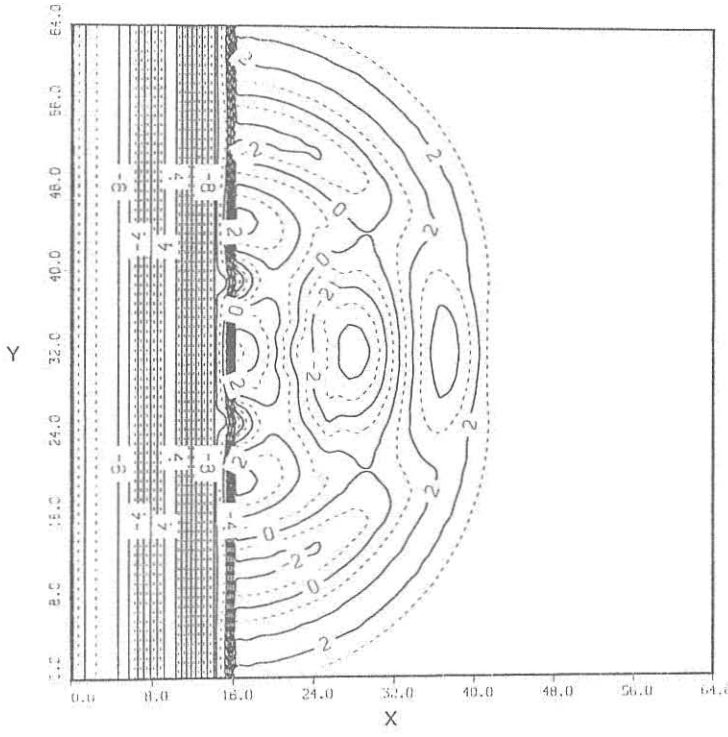

Figure 2: Spatial interference pattern of the wave amplitude in a two-dimensional wave lattice gas double-slit experiment at a given instant.

and $\sigma^2 ct \log(|\mathbf{r}|)$ for two-dimensional. Therefore, for a given number of time steps, a sufficiently large number of CA cells such that $L >> c$ and the mean wave amplitude $|\bar{U}| >> |\sigma|$, the noise is basically confined to small spatial scale for three-dimensional case and large scale wave structures remain undeformed. However, the fluctuation has stronger influence at large scales for two-dimensional.

3. Conclusions

In this report, we have presented a CA wave model for the linear wave equation. It is a many photon lattice gas system. Since the wave CA system conserves the macroscopic energy and momentum, its behavior follows a Hamiltonian dynamics. This is an essential requirement in formulating a CA wave process. It is foreseeable that more complicated wave processes may be constructed involving possibly many different kinds of nonlinear interactions. Since the CA provides a fast computational tool, many practical physical problems involving complicated geometries can be simulated.

Acknowledgements

We thank W. Mattheaus, D. Montgomery, H. Rose, and Y. T. Yan for their instructive discussions. The work is supported by the U. S. Department of Energy.

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