ELSEVIER

Computational Materials Science 18 (2000) 132–140

COMPUTATIONAL MATERIALS SCIENCE

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Cellular automata simulation of dispersion of pollutants

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Received 29 January 1999; accepted 14 August 1999

Abstract

In this work, a novel application of *cellular automata* (CA) to the analysis of pollutants dispersion in the atmosphere is presented. It includes a quick review of the mathematical background, the actual model formulation, and a simulation of a real example, showing the applicability of the software developed. © 2000 Elsevier Science B.V. All rights reserved.

1. Introduction

During the last few decades, the World has gone through an intensive economic growth along with a steady increase of population, but with an almost careless environmental control. Indeed, Nature was regarded as another asset, and environmental utilities, such as water and nutrients, that could be recycled, as well as carbon sinks, and climate control, were not considered as a part of the economic processes since their value was nil. Nevertheless, a new way of thinking looking for new alternatives against the environmental crisis has arisen [1–6]. This new vision, in fact, considers the ecological, economic, and social problems as a whole. Nowadays, simulation techniques seem to be an excellent tool for overcoming, or at least to alleviate, some of those problems. In fact, all the software developed for simulation, especially those focused for simulating physical, chemical, biological, etc., phenomena, are a necessary tool for pursuing research about pollution processes [7–9]. This is so, because it would be almost impossible, for example, to perform an experiment in vivo for analyzing the pollutants dispersion in the Mexico City's atmosphere. The possibility of a computer simulation has become almost indispensable for the understanding and prevention of some processes about water and air pollution, amongst others.

Some of the algorithms more frequently and widely applied to several scientific and technological problems are of the type known as *cellular automatas* (CA) [10–14]. These have been applied from the early developments for intelligent robots up to the study of the properties of new materials. In this work, a novel application of CA to the analysis of pollutants dispersion in the atmosphere is presented. This includes a quick review of the mathematical background, the actual model formulation, and a specific example showing the applicability of the software developed.

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0927-0256/00/$ - see front matter
PII: S0927-0256(00)00097-5

2. Mathematical background

A wide number of research works regarding air pollution have been carried out [12–22]. Some of them have been focused to the analysis of pollutants, at the molecular level, and their combinations with the natural atmosphere elements and compounds. On the other hand, there are some others focused at the dispersion phenomena, but at the microscopic level. In both cases, though, these studies allow to predict the pollutants behavior based upon mathematical models describing the phenomena, and their simulations. Clearly, because of the complexity of the models, these have to be solved numerically.

In this work, CA are the mathematical models for computer simulations trying to model Nature's behavior. The concept of CA was first introduced by Von Neumann [11] for a particular task, namely, to prove the existence of a universal computer capable of self-reproduction within a defined space. This concept has evolved into a theory leading to different types of CA, which in turn, and based upon their features, have been applied to a variety of physical phenomena, as well as biological, chemical, etc.

From the systems standpoint, an AC is a discrete dynamic system, i.e., space, time, and the system states are discrete. Each point in a regular space grid called *cell* may have any number of finite states. The cell states in the grid are updated based on a local rule, i.e., the state of a cell in a given time only depends upon its own previous state. All the cells within the grid are simultaneously updated, i.e., the whole grid state changes in discrete time steps.

A type of AC of particular interest for fluid dynamics simulation are the so-called AC lattice gas. This concept has evolved and now is applied to the simulation of sound waves, diffusion processes, viscosity effects, etc. An AC lattice gas is an example of an AC set using updated rules for fluids simulation. In this model, the grid nodes (called *lattices*) have information about the incoming and outgoing particles through a particular node. In a square grid, the node "knows" about the particles localized in the North, South, East and West.

The first AC lattice gas model, also called the HPP-model, was first introduced by Hardy [13], for studying problems related to ergodicity. Since these systems are completely discrete, they can be directly computer implemented. Thus, computer simulations with more particles with continuous values for position, velocity, and potential interactions could be performed instead of the limited real models.

The HPP-model is based upon a square grid whose nodes can be occupied by particles of some fluid. This space is discrete and, in practice, is also finite. The boundary conditions can be chosen, amongst others, of the periodic type, with backward jumps, wind tunnel type, or any other convenient way. Besides, the impulses are distributed in a discrete fashion, since all the particles are considered of unit mass and they have the same absolute velocity. Time is also discrete, since it is considered that all the particles will move to the neighboring node in a unit time. There is an exclusion principle imposed on the particles, namely, two particles cannot be simultaneously installed in the same node if their direction is identical. In a HPP square, the above means that there will be no more than four particles per node. Therefore, the state of each node can be described by a four-bit word. This is equivalent to say that the particles equilibrium-distribution is of the Fermi–Dirac type, which is consistent with the general statistical physics.

The interactions amongst particles are simple, i.e., if there are several particles in a node, then they will be considered as instantaneous local collisions. The collision rules are selected in such a way that mass and momentum are preserved. In this model, energy conservation is discarded since energy is proportional to mass.

The evolution of a lattice gas for an instant of time can be divided into two steps:

(i) *Propagation*. The particles move from their node towards their closest neighbors in the direction of their velocity.

(ii) *Collision*. The particles in the same node can change their moment if this is compatible with the invariance rules.

In Figs. 1–3, different evolution stages of an AC lattice gas is shown.

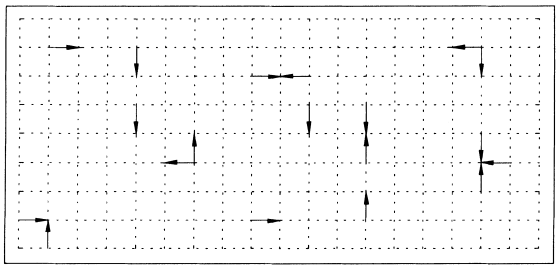

Fig. 1. At instant $t = 0$, the particles are at the nodes of a square grid.

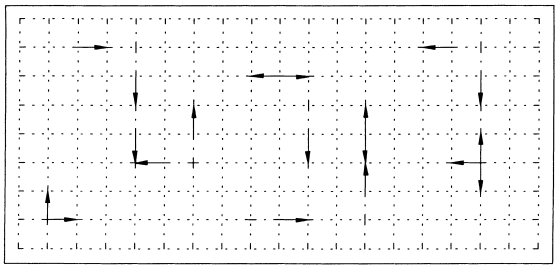

Fig. 2. At instant $t + \epsilon$, all the particles have jumped to the closest neighbor at their velocity direction.

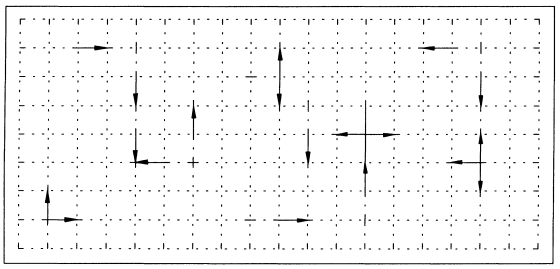

Fig. 3. At instant $t = 1$, whenever possible, the particles at the same node change their impulse.

Assuming a two-dimensional space divided into squares, in each of them can stay a maximum of four particles, with different velocities; thus, there exists 16 possible situations for the particles at any grid square. This situation is shown in Fig. 4.

Let us call E_{ij} the allowed set of positions and velocities of the grid particles; where

$$0 \leqslant E_{ij} < 1111,$$

i and j being the intersection of the ith column and the jth row. The transition phase is defined [12] as

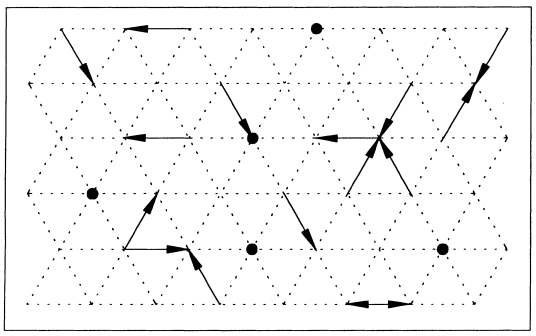

Fig. 4. Possible situations at a lattice.

$$(T_0 E)_{ij} = d_{i,j+1}\, c_{i+1,j}\, b_{i,j-1} + a_{i-1,j},$$

where T_0 represents the translation operator. Thus, the collision phase can be expressed as

$$\begin{aligned} 0101 &\quad \text{if } E_{ij} = 1010,\\ CE_{ij} &\quad \text{if } E_{ij} = 0101,\\ E_{ij} &\quad \text{otherwise,} \end{aligned}$$

C being the collision operator. Usually, after the phase collision, the bit values of each place on the grid depends upon the previous values, i.e., it is a bitmap of n bits in the grid towards n bits in each square of the same. Nevertheless, there exists some lattice gas whose collision phase is stochastic.

A last distinctive feature of the lattice gases is the conservation of some amounts linearly dependent on the bits values. In some models, the total number of particles remains as in Fig. 5, where the velocity horizontal and vertical component remain on each row and column, respectively.

Lattice gases and CA are similar, but, the trend is to keep the term lattice gas for the CA in which the metaphore of gas or particle motion can be used.

The main features of these types of models are:

(i) CA are a general paradigm for distributed computation either in vector or in parallel computers,

(ii) CA are discrete dynamic systems and can be studied through very well-known techniques, where properties such as stability, stationarity, ergodicity, etc., can be identified.

CA can represent original models for physical phenomena, being competitive with the existing

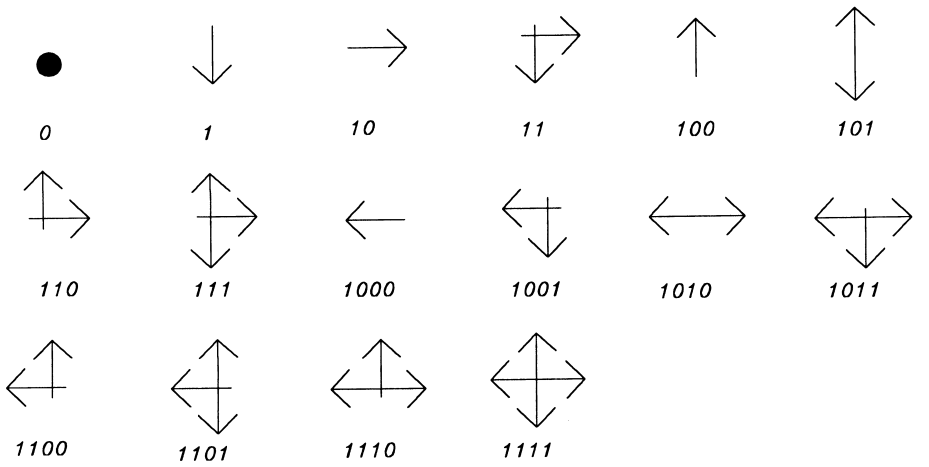

Fig. 5. Tridimensional AC.

continuous models. CA have been applied to several problems characterized for having a dynamic behavior and a substantial spatial variability. Guariso [12] propose a special formulation of CA for simulating the behavior of one pollutant in the atmosphere. This is the basis for this work, the objectives being described below.

3. Algorithm design

Based on the concept stated in [12], the main objectives of this work are:

(i) to formulate a mathematical model of pollutants dispersion, starting from the basic concepts of Physics, Chemistry, and Computation;
(ii) to develop an algorithm of CA, based on (i);
(iii) to implement the algorithm in a computer program using object-oriented programming techniques;
(iv) to develop a software for the optimal execution on a PC;
(v) to set the background for future developments on the subject, highlighting the endeavor a computation engineer and materials science could have.

Each element of the CA, $C_{ijk}(t)$, is identified by its position i, j, and k, along the X-, Y-, and Z-axes, respectively, and C represents the cell state at time t.

The AC cell state represents some pollutant concentration, which is represented by the number α, with $0 \leqslant \alpha \leqslant M$, where M is the pollutant maximum concentration in the cell. The finite automata of each cell is represented by an updated rule. With this rule, each cell state is computed, according to the state values of its neighbor cells, as shown in Fig. 6.

The update rule is affected by the following physical factors:

Gravity. This produces the mass (amount of pollutant) interchange between cells lying in the same column. This balance of mass can be modelled as

$$D_{\mathrm{g}}C_{ijk} = \mathrm{g}(C_{ijk-1} - C_{ijk}), \tag{1}$$

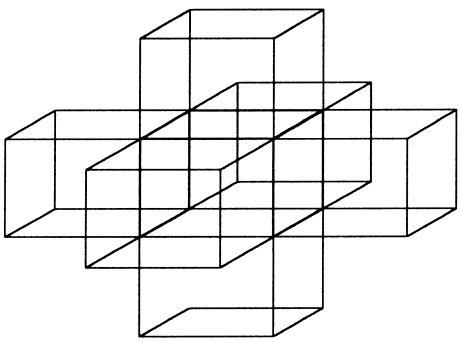

Fig. 6. Proposed CA with its six neighbor cells.

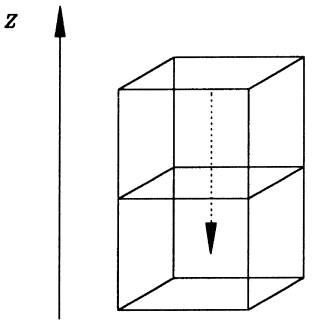

Fig. 7. Gravity effect.

where D_g is the pollutant concentration variation in the cell, due to gravity, and considered in a unit time; g is the gravity acceleration (9.81 m/s^2). This effect is shown in Fig. 7.

Diffusion. This produces mass interchanges between neighbor cells due only to concentration gradients. It is assumed that there exists an isotropic diffusion, i.e., the mass diffusion is the same in all the three directions. The relation for mass balance due to diffusion is

$$\begin{aligned} D_d C_{ijk} = {} & dz\,(C_{ijk-1} - C_{ijk}) + dy\,(C_{ij-1k} - C_{ijk}) \\ & + dx\,(C_{i-1jk} - C_{ijk}) \\ & + dz\,(C_{ijk+1} - C_{ijk}) \\ & + dy\,(C_{ij+1k} - C_{ijk}) \\ & + dx\,(C_{i+1jk} - C_{ijk}). \end{aligned} \tag{2}$$

Transport. This is determined by the wind velocity. The mass balance due to transport is

$$\begin{aligned} D_t C_{ijk} = {} & w_i(C_{ijk-1} - C_{ijk}) \\ & + w_j(w_i(C_{ij-1k} - C_{ijk})w_k(C_{i-1jk} - C_{ijk}), \end{aligned} \tag{3}$$

where w_i, w_j, and w_k are the wind speed parallel to the X-, Y-, and Z-axes, respectively, as shown in Fig. 8.

After algebraic manipulations of Eqs. (1)–(3), one obtains

$$\begin{aligned} DC_{ijk} = {} & \alpha C_{ijk} + \beta C_{ijk-1} + \gamma C_{ij-1k} + \psi C_{i-1jk} \\ & + d_x C_{i+1jk} + d_y C_{ij+1k} + d_z C_{ijk+1}, \end{aligned} \tag{4}$$

where

$$\begin{aligned} \alpha &= -g - w_i - w_j - w_k - 2d_x - 2d_y - 2d_z, \\ \beta &= d_z, \\ \gamma &= w_j + d_y, \\ \delta &= w_k + d_x. \end{aligned}$$

Eq. (4) is the update rule, which determines the cell internal states of the proposed CA, and was used in the case presented below. It is worth mentioning that Eq. (4) differs slightly from the one proposed by Guariso [12] in the sense that the β factor lacks an equivalent in Guariso's.

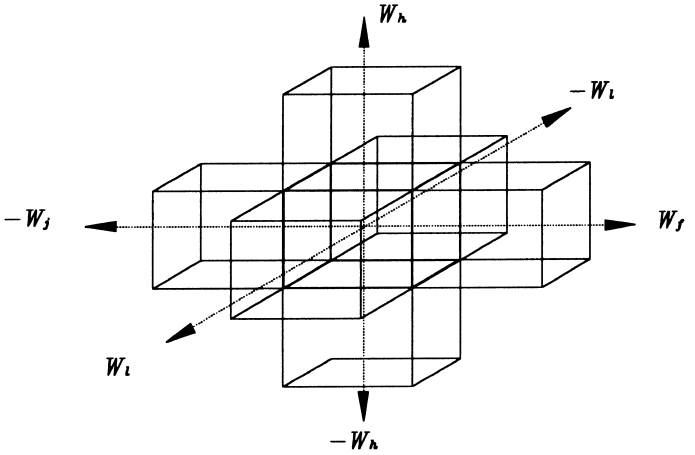

Fig. 8. Wind speed in the three directions move cells parallel to the same direction.

4. Results and discussion

For testing the proposed CA, three real mexican petrochemical complexes, along the Gulf of Mexico shoreline [23], were selected for studying the effects of air-dispersed pollutants on the steel structures of those complexes. This was done placing controlled steel plates, for collecting sulfides, at each of the selected places. A typical test layout is shown in Fig. 9. After an exposure period, the plates were analyzed in terms of the loss of weight, color, and corrosion mechanisms, as well as the presence of sulphur, chloride, and phosphorous. The concentration distributions for four test stations (C_1–C_4) are displayed in Table 1 and shown in Fig. 10.

The high value shown for the C_3 station, is justified because there are crude-oil tanks close by which produce HS. Similarly, for C_4 there is a cooling tower producing a heavy sprinkle with chloride and sulphur. For testing our model, we only considered the diffusion phenomenon of sulphur dioxide.

Table 1
The concentration distributions for four test stations (C_1–C_4)

Station no.	Sulphur dioxide
C_1	8.03
C_2	8.72
C_3	24.53
C_4	9.42

The first approach for the main features of the CA can be summarized as:

- Dimensions [14, 25, 9].
- Station C_3 is located at [11, 22, 1].
- Wind speed is constant from South to North, and the dispersion towards East is also constant.
- The cero cell is located just below the crude-oil tanks, at [11, 22, 0].
- The cells located in the region [8, 15, 0] to [9, 16, 2] were assigned with a higher α value than others for taking into account the sprinkle produced from the cooling tower, as described earlier.
- The pollutant maximum concentration was set to $M = 100 \times 10^6$.

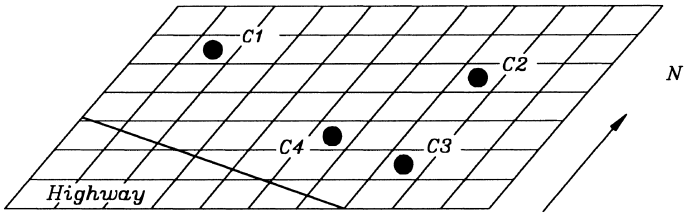

Fig. 9. Layout of the testing plates.

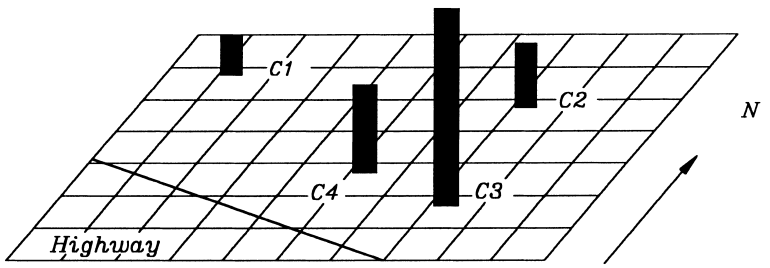

Fig. 10. Distribution of sulphur dioxide on the testing plates.

- The initial state of cell [11, 22, 1] was 90×10^6 (arbitrary units).
- The number of iterations was 45.

After several trials, the final approximation for starting the simulation is shown in Figs. 11 and 12, where the windows displayed in Fig. 12 correspond to planes parallel to the YZ-plane and the coordinate X being displayed on the window title.

Clearly, the most crucial part of the model is the parameters calibration, according to the corresponding CA update rule. Moreover, knowing the effects of each of them on the CA allows for a quick final approximation. Once the model tuning is achieved, then it is possible to vary the update rule parameters, for example:

(i) by changing the α value, it is possible to simulate in the region [8, 15, 0] to [9, 16, 2] the effect of a cooling tower sprinkle increase, or if there is no cooling tower at all ($\alpha = 0$),
(ii) changes of d_z, this would mean to consider heavier particles,
(iii) to increase or decrease the wind velocity,
(iv) to place several pollution sources,
(v) to assign cero values to a specific region for simulating terrain irregularities, or obstacles such as walls, mountains, etc.

The aforementioned variations allow for a high flexibility of the CA behavior.

5. Conclusions

Software development for simulation, especially those focused to physical and chemical phenomena, requires the interaction of several scientific and

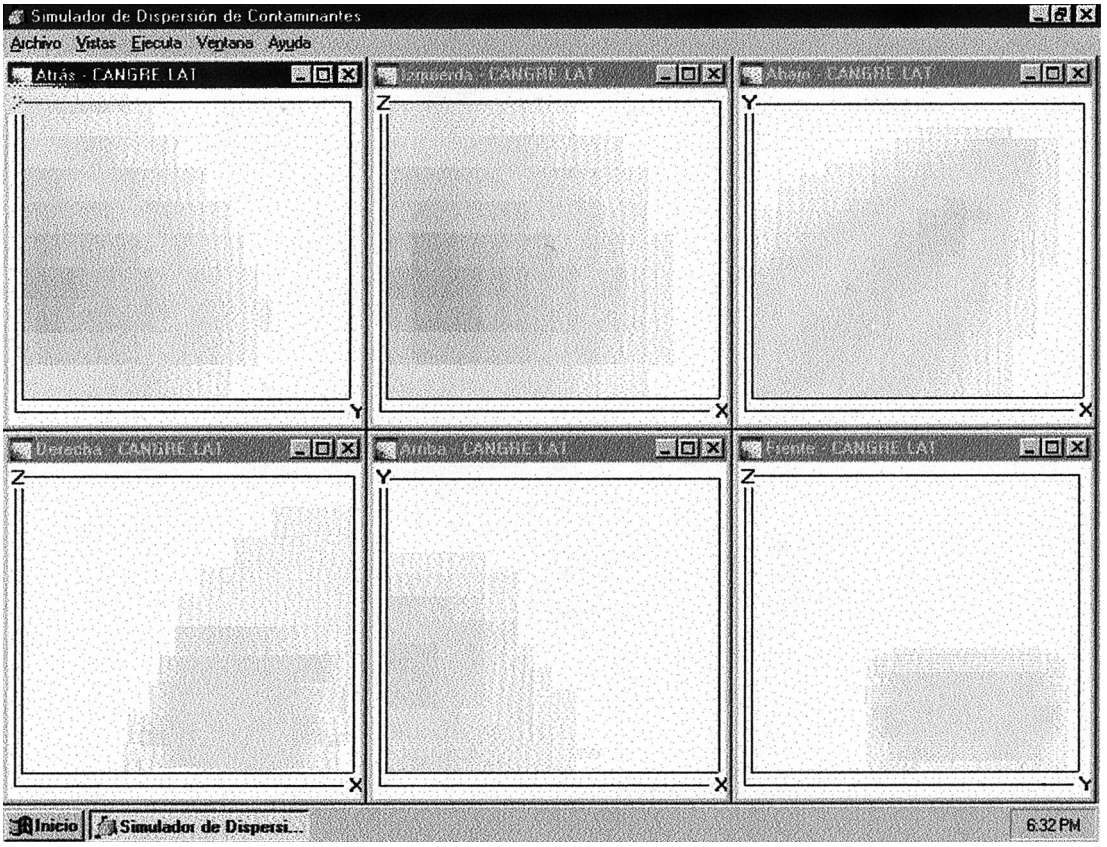

Fig. 11. Final approximation for starting the simulation.

Fig. 12. CA-axes layout with respect to one of the sampled petrochemical complex.

technological disciplines. Indeed, the one presented in this work, was based on a theoretical basis of a special type of dynamic systems known as CA, and, moreover, required object-oriented programming. The main features of the software presented in this work are:

- It was built on a hardware platform for PC systems. This allows to be used at research institutions and universities lacking larger computer facilities.
- The simulator for pollutant dispersion works on a standard graphics environment, is user friendly through dialog boxes, menus, windows, etc.
- The use of object-oriented programming allows for greater flexibility in future versions.
- The process speed and display of results is essential in any simulation program. In the particular one presented herein, the program uses the whole system memory and has an excellent response time, even though number crunching.

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