MODELLING CONSERVATION QUANTITIES USING CELLULAR AUTOMATA

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Abstract. Cellular automata (CA) have proven to be a suitable tool in modelling tasks, specially, when the underlying procedures of a model are difficult to be expressed in mathematical terms. Thus, being a soft tool CA are often be referred as having not the same accuracy as classical methods. In this paper it will be shown, that CA can show pretty accuracy depending on the underlying problem, and that CA are capable to maintain also conservation quantities.

Based on a mathematical model which describes the migration of pollutants in the form of actinoides (radioactive heavy metals) in soil, the conservation of the amount of substance was shown by particle counting. The implementation was performed by taking the transport equation and some other relevant migration processes (sorption, radioactive decay) and transforming them into an automata rule. In the following the migration of different actinoides was observed. The spreading of the pollutants as well as the migration of their progenies were summarised all time at all cells. Soon it was seen that the total amount of pollutants present in the model was always constant. Taking the amount of substance by known molar mass of each concerning nuclide into account also mass conservation was shown by this model.

Moreover, as long a any conservation quanitity like, mass, energy, momentum, anugular momentum, etc. can be discretised or at least reasonable subdivided into smaller parts, CA are capable to maintain them throughout a modelling process.

1 Introduction

Cellular automata (CA) have been proven to be a suitable tool in modelling tasks, specially, when the underlying procedures and processes are difficult to express in mathematical terms. This might be due to a lack of a mathematical theory for the specific problem or too many uncertain parameters left. Thus, modelling such tasks by classic methods (white-box) model might give big problems and usually black-box models are used instead. The inner structure of black-box models is often unknown or can't be described in detail, but at least the behaviour and interactions of the system are well known.

The characterisation of a contaminated area by actinoides (heavy metals, starting in the periodic system of the elements at thorium and ends at lawrencium, all of them are radioactive) builds up the basis for this modelling task. The underlying dynamics of a complex system like the migration of such pollutants is not known in detail. Indeed, the most important processes like diffusion and advection can be described mathematically very well by their respective PDEs. But there're also other processes, which influence migration and dispersion significantly, i.e. sorption. Although sorption is a well observed process, it is far too complicated to be expressed by a simple mathematical construction, like a formula . Thus, modelling the migration of actinoides in contaminated soil is far too imprecise for a white-box model. But as long as the behaviour and interactions of processes like sorption are somewhat known, a black-box model, like using a CA, would be sufficient enough.

The migration model was to be compared to a contaminated area at a former nuclear facility. Clearly speaking, the concerning site was contaminated by a mixture of different plutonium isotopes [plutonium atoms with different mass numbers: plutonium-238 (^{238}Pu), plutonium-239 (^{239}Pu), plutonium-240 (^{240}Pu), and plutonium-241 (^{241}Pu)]. By characterising that site in detail by taking soil samples on a 1m x 1m sampling grid and analysing them in a suitable laboratory, also the also the progeny of ^{241}Pu americium-241 (^{241}Am) was detected. Due to the fact that there already was a sampling grid, a modelling strategy that works also on the base of a grid was chosen in order to get big advantages when comparing both results.

2 Basic principles of the migration model

Modelling the contamination of contaminated sites the understanding of processes of migration and dispersion are essential. Although contamination may originally be dispersed, secondary processes may concentrate, fractionate or otherwise distribute pollutants, or radioactive material.

There are several linked processes which can influence the migration ability of pollutants in any medium. Additionally, the radioactive decay chains of the concerning pollutants have to be considered in this computer model. The most important and best known processes for the migration of any pollutant are diffusion and advection. Thus, migration processes which only proceed via these can be implemented perfectly to a white-box model.

Even considering radioactive decay can be regarded in a white-box model due to its mathematical description by an ODE.

Central processes for the migration of pollutants like actinoides in soil are matrix diffusion, the distribution due to groundwater or leakage water by advection, sorption and radioactive decay. These migration processes provide the key terms for the migration equation for the underlying model. Figure 1 shows the pattern of the migration model, its key terms and their interactions. There're also other, secondary processes, but their influence is far too weak to be taken into account. In the following all key processes are described shortly.

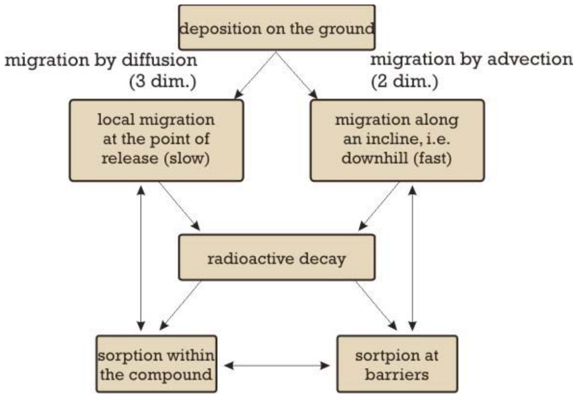

Figure 1. Pattern of the migration model for actinoides in contaminated soil. Driving forces are diffusion and advection, but sorption blocks the migration, but also radioactive decay has always be considered.

Diffusion. Diffusion is a physical equilibirum process, whereby particles of areas of higher concnetration migrate by Brownian motion to regions of lower concentrations in order to achieve equilibrium. The *3-dim.* equation is also known as Fick's Law and can be expressed by an experimentally derived diffusion constant *D* in the diffusion equation.

$$\frac{\partial c}{\partial t} = D \cdot \left(\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2} + \frac{\partial^2 c}{\partial z^2} \right)$$

Advection. Advection is a transport mechanism of a substance or a conserved property with a moving fluid. The fluid motion in advection is described mathematically as a vector field, and the material transported is typically described as a scalar concentration of substance, which is contained in the fluid. Combining the processes of diffusion and advection gives the transport equation.

$$\frac{\partial c}{\partial t} = D \cdot \frac{\partial^2 c}{\partial \vec{x}^2} - \vec{v} \frac{\partial c}{\partial x}$$

Sorption. Sorption refers to the action of both absorption and adsorption taking place simultaneously. As such it is the effect of pollutants being incorporated into a material of a different state and adhering to the surface of another molecule. Sorption is a far too difficult process to be described in one simple formula. Moreover, al lots of submodels have been presented in order to get an adequate description of the sorption behaviour of a system. For the underlying work the concept of the equilibrium sorption model (K_d model) was used und results in a retardation factor *R* for the diffusion constant *D* and fluid velocity *v*. Thus, the migration equation of actinoides in soil is given:

$$\frac{\partial c}{\partial t} = \frac{D}{\underbrace{1 + K_d}_{R}} \cdot \frac{\partial^2 c}{\partial x^2} - \frac{\vec{v}}{\underbrace{1 + K_d}_{R}} \cdot \frac{\partial c}{\partial t}$$

Radioactive Decay. Radioactive decay is the process in which an unstable atomic nucleus loses energy by emitting ionizing particles and radiation. Radioactive decay can be expressed mathematically by 1st order ODE which gives the decrease of a number of a radio nuclide *N* during time *t* due to its decay constant λ.

$$N(t) = N(t_0) \cdot e^{-\lambda \cdot t}$$

3 CA and CA-Rules

A cellular automaton (CA) is a discrete model studied in computability theory, mathematics, theoretical biology and microstructure modelling. It is of a downright simple construction. A CA consists of a regular grid of cell from 1 to n dimensions, each in one of a finite number of states. Time is discrete, and per definition, the state of a cell at time t t is a function of the states of a finite number of cells (called its neighbourhood) at time *t-1*.

The neighbourhood is defined by a selection of cells relative to the considered cell, and does not change all the time. Every cell of the CA has the same updating rule, based on the states of the cell's neighbourhood. Each time, the updating rule is applied to the automaton a new generation in time is created.

For the spreading of actinoides by diffusion the *von-Neumann neighbourhood* was chosen. Heavy metals like these elements have shown a weak affinity towards diffusion equilibrium. Thus a weak ability for diffusive migration has to be implemented in the model by a small diffusion constant, see figure 2 (left).

For dispersion by advection, some kind of a simplified *Moore neighbourhood* was chosen, because convection proceeds fast along a natural incline. The vector component, which has the same direction as the natural incline, also drives the strongest force for advection, see figure 2 (right).

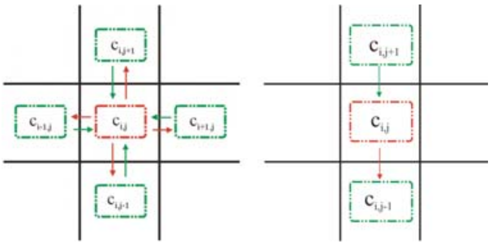

Figure 2. Diffusion takes place within a von-Neumann neighbourhood (left), whereas the migration process of advection is performed within a simplified Moore neighbourhood (right).

First of all, the migration of any pollutant by neglecting radioactive decay will be considered. To translate the migration equation to an automata rule it has to be transformed to a discrete form by formal integration. The main principle of the implementation lies in the conservation of the amount of substance. The conservation of the amount of substance is quite a seldom used conservation quantities, but using it shows several advantages. Taking the atomic mass number of every concerning nuclide into account the amount of substance and mass can always be exchanged in the model. Likewise, by taking Avogadro's number (1 mole holds 6.002 10^{23} particles) into account, it is possible to exchange concentration and mass by the number of particles and can therefore be easily compared to lab results given in activity concentration. Performing integration, the concentration *c* was replaced by the number of particles *N*, as explained above.

$$c(x_0, t=1) = \int dt \left(\frac{D}{R} \cdot \frac{\partial^2 c}{\partial x^2} - \frac{\vec{v}}{R} \cdot \frac{\partial c}{\partial x} \right)$$

$$N(t) = N(t-1) \cdot (1 - d - v)$$

Now, the number of particles in a certain cell changes by time following the rule above. At this point, the radioactive behaviour is not yet considered, i.e. this equation is suitable for any pollutant in soil. Considering the different neighbourhoods for diffusion and advection as shown in figure 2, the CA-rule can be determined as:

$$N_{diff}(x,y,t+1) = N(x,y,t) - 4dN(x,y,t) + d[N(x-1,y,t) + N(x+1,y,t) + N(x,y-1,t) + N(x,y+1,y)]$$

$$N_{adv}(x,y,t+1) = (1-v) \cdot N(x,y,t) + N(x,y+1,t)$$

4 Generating the Migration Model

A simple CA consists of a regular grid of cell from *1* to *n* dimensions, each in one of a finite number of states. For generating the migration model, it was necessary to design the CA by 7 regular grids all of them arranged one of the top of the other. In the following, each of them is named as layer, see figure 3. Every layer has the mathematical appearance of a matrix. Thus, all spreading via the CA-rule can be performed as comparable simple matrix manipulations. Each layer represents one of the concerning radio nuclides, i.e. one layer represents ^{241}Pu, one represents ^{241}Am, and so on. And each layer only performs these manipulations which are regarded to the concerning nuclide.

Now radioactive decay can be taken into account, therefore, the decay chains have to be considered. ^{241}Pu decays to ^{241}Am, which decays to ^{237}Np, which half-life is too long to be considered any more in the model. The other decay chains were considered in a similar way. Now, observing the migration of a certain ^{241}Pu particle on the ^{241}Pu-layer. The moment, the ^{241}Pu-particle decays to ^{241}Am, the particle is shifted towards the ^{241}Am-layer, where further migration of that particle proceeds, and so forth.

The uppermost layer represents the contaminated area. There, a mixture of different radio nuclides is dispersed, but the migration itself of each nuclide is calculated in the respective layer, and shifted due to radioactive decay to the appropriate layer. Summarising all nuclides all over the time in the uppermost layer therefore gives the total number of particles in the whole system all the time. Observing the total amount of particles all over the time has shown that the number of particles in the system stayed constant all over the time. Doing reverse calculation in additional layers in order to get the amount of substance or in order to get total masses, also these quantities are preserved over all the time.

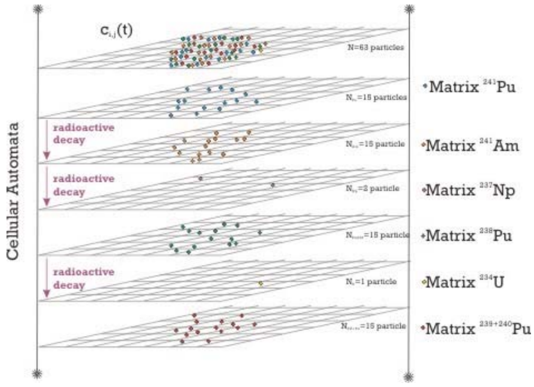

Figure 3. Schematic diagram of the CA that models the migration model for actinoides in soil. The topmost layer represents the contaminated area itself and holds the conservation quantities of the model by summarising all particles all the time. The dispersion processes are calculated for each nuclide separately in the respective layer. Actinoides can change from one layer to another by radioactive decay.

As the migration model consisted of up to 7 layers (matrices), it was convenient to implement this model to MATLAB. There, all manipulations could be performed easily, especially, the summing over all nuclide-layers in order to observe a possible drift of conservation quantities. But these quantities stayed constant, not even a numerical drift, caused by the discretisation of the PDE was observed.

The computer model about the migration of radio active heavy metals in soil was compared to a truly contaminated site. It has been shown, that by choosing appropriate migration parameters (diffusion constant, fluid velocity, retardation factors) the computer model suits very well to reality, see figure 4.

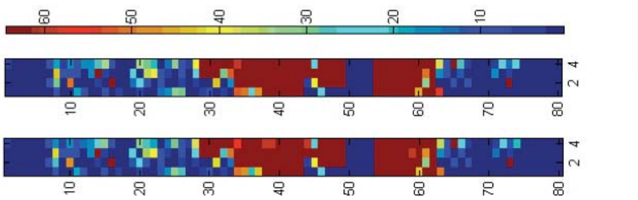

Figure 4. The picture shows the comparison of results by the migration model (top) and by laboratory analyses (bottom).

5 Conclusion

Observing the migration model it was easily seen that CA are also capable to maintain conservation quantities like amount of substance and mass. The idea is subdividing the whole amount into suitable smaller parts. Thus, a conservation quantity has to be discretised or at lest reasonable subdivided into smaller parts (quantised) in order to achieve a good working automata rule. The only precondition for observing conservation quantities in such systems is the discretisation of the quantity to be conserved prior its implementation to the CA-rule. Also conservation quantities like momentum, energy, angular momentum and spin can be modelled by CA as long as they can be reasonable portioned to the cells of the CA.

6 References

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