

Multi-physics Modeling Using Cellular Automata

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This paper proposes a new modeling and solution method that is relatively simple yet powerful enough to handle complex multi-physics problems. The new methodology is based on a combination of cellular automata, finite difference, and analytical analysis concepts. The basic idea is to construct a cascading sequence of simple, explicit rules of evolution, rather than attempt to solve complicated partial differential equations. The resulting scheme is computationally explicit yet numerically stable. In addition to significant modeling flexibility, the cellular automata environment lends itself to extremely efficient computational algorithms and hardware implementation due to its inherent use of local rules and potential for parallel computation.

The power and flexibility of the method is demonstrated by developing solutions for a general transport process consisting of elementary processes due to diffusion, advection, reaction kinetics, and external interaction. Explicit and numerically stable rules for each of these elementary processes are developed. Case studies produce physically realistic and numerically accurate solutions for complex processes. Numerical experiments show that the method is highly accurate if the time step is sufficiently small.

The value of the method is that a library of rules for simple, elementary processes can be derived individually. These processes can be assembled in a modular manner in any combination to create models for complex processes. The method is currently being used in a number of applications, including a study of complex thermal/mechanical phenomena at the sliding contacts between rubbing surfaces.

1. Introduction

Mathematical modeling of complex systems is important for numerous reasons, including the development of a fundamental understanding of the underlying physics, prediction of natural phenomena, identification of critical intrinsic parameters (i.e., the inverse problem), and optimization of particular processes. However, simulations of complex processes

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are extremely challenging, as they often involve multi-physics phenomena in complex heterogeneous systems. To address this challenge, this work offers a new generalized approach to modeling and analyzing simulations of multi-physical phenomena. Implementing such complex models using traditional procedures (e.g., finite element and finite difference methods) is often not practically feasible due to excessively long computation times and limited multi-physical or adaptive capabilities.

The objective of this paper is to develop and implement an algorithm for general multi-physics models of complex processes. In order to attain this goal, a rule-based solution method is developed that combines fundamental ideas from traditional finite difference methods, analytical analysis, and cellular automata. The unique feature of this solution methodology is that rather than attempting to develop equations for entire complex processes, computationally explicit, yet numerically stable rules for elementary physical processes are developed individually. These elementary rules are then assembled in a cascading sequence at each time step to form a complete process. The cascading sequence of explicit rules is applied to the state variables to transform them from one state to the next.

2. The fundamental idea

The current solution method is a unique combination of fundamental ideas from finite differencing [1], analytical analysis, and cellular automata [2]. The basic idea is to split complex processes into simpler, elementary processes, as first suggested by Strange [3]. Each elementary process is advanced in a discrete manner in time using a computationally explicit yet numerically stable rule. The total process is then assembled by applying each elementary rule in a cascading, sequential manner.

2.1 General processes

A collection of state variables is represented by the matrix $\mathbf{U}$. These state variables change with time due to a total process consisting of N elementary processes. The rate equation for the complete process is represented as

$$\frac{\partial \mathbf{U}}{\partial t} = \sum_{n=1}^N P_n[\mathbf{U}]. \quad (1)$$

Here P_n represents one of the elementary processes, such as diffusion, convection, external interactions, chemical reactions, or any other physical phenomena. This total process could be quite complex and equation (1) could be difficult to solve. However, each individual process is in general much easier to deal with.

2.2 Elementary processes

The rate equation, considering process n only is

$$\frac{\partial \mathbf{U}}{\partial t} = P_n[\mathbf{U}]. \quad (2)$$

This elementary process is applied over a spatially discretized cellular grid or network of cells and is advanced in discrete time steps. The state variable vector containing a list of the $\mathbf{U}$ values at time step k is denoted as $\mathbf{U}^k$. The rule for advancing the state variable vector $\mathbf{U}^k$ over one time step due to elementary process n only is represented symbolically as

$$\mathbf{U}^{k+1} = \Phi_n[\mathbf{U}^k] \quad (3)$$

where Φ_n is the specific rule corresponding to process n only. Rules for each of the elementary, simpler processes are developed individually and collected in a library of rules, as described in section 4.

2.3 Construction of complex processes

Once rules for elementary processes have been developed, a complex process consisting of N elementary processes is constructed as a cascade of the elementary processes in the form,

$$\mathbf{U}^{k+1} = \Phi[\mathbf{U}^k] = \Phi_N[\dots \Phi_2[\Phi_1[\mathbf{U}^k]] \dots]. \quad (4)$$

The interpretation of this total rule is as follows: The rule for Process 1 is performed on the state variable array from the previous time step $\mathbf{U}^k$, disregarding all other physical processes. The rule for Process 2 is performed on the state variable array from the previous intermediate step, again disregarding all other physical processes. This sequence is continued until the last rule for Process N is performed on the state variable array from the previous intermediate step. The result from this last process is then the state variable array at the new time level, $\mathbf{U}^{k+1}$.

This strategy can be applied to a model containing any combination of physical processes. The accuracy of this scheme depends on three major factors: (1) the accuracy of the elementary rules, (2) the accuracy of the splitting and reconstruction process, and (3) the time step.

3. Transport processes

3.1 General transport processes

The general modeling and analysis process described in section 2 is now applied to basic transport processes. A medium is considered that contains a collection of interacting state variables, denoted by the vector $\mathbf{U}$. The individual state variables could be concentrations of chemical

components, energy density, momentum, or any other quantity needed to describe the state of a system. The dynamics of these state variables are governed by transport due to the following fundamental mechanisms: (1) advection due to bulk motion of the medium, (2) diffusion, (3) reaction kinetics, and (4) interactions with an external environment. Conservation of species applied to a differential volume produces the following set of coupled partial differential equations for the rate of change of the state variables,

$$\frac{\partial \mathbf{U}}{\partial t} = -\mathbf{V} \cdot \nabla \mathbf{U} + \mathbf{D} \cdot \nabla^2 \mathbf{U} + \mathbf{R}[\mathbf{U}] + \mathbf{S}[\mathbf{r}, t, \mathbf{U}] \quad (5)$$

where $\mathbf{r} = x\hat{\mathbf{i}} + y\hat{\mathbf{j}} + z\hat{\mathbf{k}}$ is the position vector, t is time, $\mathbf{V} = V_x\hat{\mathbf{i}} + V_y\hat{\mathbf{j}} + V_z\hat{\mathbf{k}}$ is the velocity vector, $\mathbf{D}$ is the diffusivity (m^2/s), $\mathbf{R}$ describes the reaction kinetics (typically due to chemical or biological processes), and $\mathbf{S}$ is the effect of the interactions with an external environment.

Transport processes are often modeled using variations of equation (5). Although such a formulation is quite general, analytical solutions are usually not possible, except for certain classes of linear models. Direct numerical solutions using finite difference (FD) and finite element (FE) are always possible in principle, but transient, multidimensional, nonlinear problems involving a large number of state variables can be computationally prohibitive. As a result, the modular, rule-based solution strategy proposed in this paper is applied.

■ 3.2 Elementary transport processes

The general transport equation (5) is split into elementary processes, described mathematically by the following rate equations:

$$\text{External interaction: } \frac{\partial \mathbf{U}}{\partial t} = \mathbf{S}[\mathbf{r}, t, \mathbf{U}] \quad (6)$$

$$\text{Advection: } \frac{\partial \mathbf{U}}{\partial t} = -\mathbf{V} \cdot \Delta \mathbf{U} \quad (7)$$

$$\text{Diffusion: } \frac{\partial \mathbf{U}}{\partial t} = \mathbf{D} \cdot \nabla^2 \mathbf{U} \quad (8)$$

$$\text{Reaction kinetics: } \frac{\partial \mathbf{U}}{\partial t} = \mathbf{R}[\mathbf{U}]. \quad (9)$$

The idea proposed in this work is to develop solutions for these elementary processes individually and construct complex phenomena from combinations of the basic processes.

■ 4. Rules for the elementary processes

In order to accurately and conveniently compute solutions to complex problems, rules must be developed for the simpler elementary physical

processes. Each rule is required to have the following attributes:

1. Physically realistic
2. Computationally explicit
3. Numerically stable.

Since the elementary processes are so much simpler than the total, complex process, rules satisfying the given criteria are possible. Rules for the four elementary processes given by rate equations (6) through (9) are developed next.

■ 4.1 External interactions

The interaction with an external environment could cause a change in the state of the system. This type of interaction typically involves the interaction of each cell individually with the environment, with no direct effects due to adjoining cells in the network. The general rate equation for such an effect is represented by equation (6). The physical effects of external interaction are embodied in the particular form chosen for the term $S[r, t, U]$. Quite often, the state variable U diminishes in proportion to its magnitude with proportionality factor H . In addition there could be a direct gain or loss g , which is typically independent of the state variable. A model that incorporates these effects is the linear form

$$\frac{\partial U}{\partial t} = S[r, t, U] = -H \cdot U + g. \quad (10)$$

The rule for advancing the state variable over a time increment Δt can be immediately deduced from the solution of this linear ordinary differential equation as

$$U^{k+1} = \Phi_{\text{ext}}[U^k]$$

where

$$\Phi_{\text{ext}}[U] = U \exp[-H \cdot \Delta t] + \frac{g}{H}(1 - \exp[-H \cdot \Delta t]) \quad (11)$$

If the interaction term is a nonlinear function of the state variable, a linearized form using a Taylor series can be used to bring it into the form of equation (10). Also, the effect of boundary conditions on the end cells can easily be included using this rule.

■ 4.2 Advection

The advection effect is due to transport by bulk motion. For motion in only one direction, the general three-dimensional equation (7) becomes

$$\frac{\partial U}{\partial t} = -V \frac{\partial U}{\partial x}. \quad (12)$$

Since this differential equation has a traveling wave solution of the form $U(x, t) = f(x - Vt)$, a simple and physically correct rule for advancing

the state variable is

$$\mathbf{U}^{k+1} = \Phi_{\text{adv}}[\mathbf{U}^k]$$

where

$$\Phi_{\text{adv}}[\mathbf{U}] = \text{Rotate}\left[\mathbf{U}, \frac{\mathbf{V}\Delta t}{\Delta x}\right]. \quad (13)$$

Here the $\text{Rotate}[\mathbf{U}, n]$ function rotates the $\mathbf{U}$ vector n places to the right. If $\mathbf{V}\Delta t/\Delta x$ is not an integer, the rounded value gives a suitable approximation. Alternative rules involving fractional portions for non-integer values of $\mathbf{V}\Delta t/\Delta x$ can easily be formulated, however, some degree of artificial diffusion would be introduced.

For multidimensional problems, the previous one-dimensional rule can be immediately extended in the form

$$\Phi_{\text{adv}}[\mathbf{U}] = \text{Rotate}\left[\mathbf{U}, \left\{\frac{\mathbf{V}_x\Delta t}{\Delta x}, \frac{\mathbf{V}_y\Delta t}{\Delta y}, \frac{\mathbf{V}_z\Delta t}{\Delta z}\right\}\right]. \quad (14)$$

■ 4.3 Reaction kinetics

For chemical and biological applications, a reaction term could be present, modeled mathematically by the function $\mathbf{R}[\mathbf{U}]$ in equation (9). Usually this term is of a nonlinear nature and as a result a convenient rule based on the analytical solution of equation (9) is impossible to find. However, a first-order Taylor series expansion about the current state variable provides a suitably accurate rule for most cases, particularly for small enough time steps. Equation (9) is approximated as

$$\frac{\partial \mathbf{U}}{\partial t} = \mathbf{R}[\mathbf{U}] \approx \mathbf{R}[\mathbf{U}^k] + (\mathbf{R}')^k(\mathbf{U} - \mathbf{U}^k) \quad (15)$$

where $\mathbf{R}' = d\mathbf{R}/d\mathbf{U}$. This linearized equation can be solved to provide a rule for any desired reaction kinetics. The rule is

$$\mathbf{U}^{k+1} = \Phi_{\text{react}}[\mathbf{U}^k]$$

where

$$\Phi_{\text{react}}[\mathbf{U}] = \mathbf{U} \exp[\mathbf{R}'\Delta t] - \left(\frac{\mathbf{R}[\mathbf{U}] - \mathbf{R}' \cdot \mathbf{U}}{\mathbf{R}'}\right)(1 - \exp[\mathbf{R}'\Delta t]). \quad (16)$$

A classic example of the reaction kinetics effect is the logistic model [4,5] used to describe growth in biological systems or autocatalytic reactions in chemical systems. The model is

$$\begin{aligned} \frac{\partial \mathbf{U}}{\partial t} &= \mathbf{R}[\mathbf{U}] = \mathbf{A} \cdot \mathbf{U} \left(1 - \frac{\mathbf{U}}{\mathbf{B}}\right) \\ \mathbf{R}'[\mathbf{U}] &= \mathbf{A} \left(1 - \frac{2\mathbf{U}}{\mathbf{B}}\right) \end{aligned} \quad (17)$$

where $\mathbf{A}$ is a growth rate parameter and $\mathbf{B}$ is the species carrying capacity.

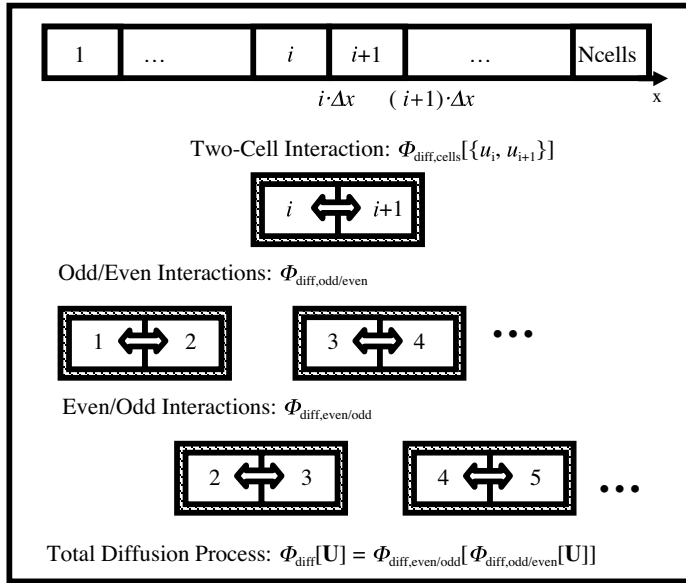


Figure 1. Algorithm used for the diffusion process.

■ 4.4 Diffusion

A simple rule satisfying all the requirements for diffusion is challenging. In fact, there are numerous alternatives that simulate the diffusion phenomena to some degree of realism. For instance, one could simply set the concentration of a cell equal to the average concentration of its adjoining neighbors at the previous time level. Although convenient, such schemes tend to over- or underestimate the diffusion effect. In addition, they violate basic conservation laws for networks with cells of variable capacity.

As a result, a rule depicted schematically in Figure 1 has been developed. The idea is to let every contacting pair of cells take turns interacting individually. Once a physically realistic rule for a two-cell interaction has been developed, that rule is applied first to all the odd/even pairs and then applied to all the even/odd pairs. This parallelizes the diffusion process as much as possible while retaining the required attributes.

The key to the success of this scheme is the two-cell interaction for a typical pair of cells, i and $i+1$. The diffusion-only relation, equation (8), is applied to a typical cell i and integrated or averaged over the cell to produce

$$\Delta x \frac{\partial u_i}{\partial t} = D \cdot \left(\left(\frac{\partial u_i}{\partial x} \right)_{i\Delta x} - \left(\frac{\partial u_i}{\partial x} \right)_{(i-1)\Delta x} \right). \quad (18)$$

Since we are treating each physical effect individually, cells i and $i+1$ are considered to be isolated except for their interaction with each other.

Thus, the interaction with cell $i - 1$, given by the flux at $x = (i - 1)\Delta x$ is zero. In addition, a simple finite difference approximation is used to estimate the flux at $x = i\Delta x$. The resulting equation is

$$\Delta x \frac{\partial u_i}{\partial t} = D \cdot \left(\frac{u_{i+1} - u_i}{\Delta x} \right). \quad (19)$$

In a similar fashion, the diffusion equation for cell $i + 1$ is

$$\Delta x \frac{\partial u_{i+1}}{\partial t} = -D \cdot \left(\frac{u_{i+1} - u_i}{\Delta x} \right). \quad (20)$$

Equations (19) and (20) constitute two coupled linear ordinary differential equations describing the dynamics of u_i and u_{i+1} due to diffusion. The analytical solution provides the desired two-cell diffusion rule as

$$\{u_i, u_{i+1}\}^{k+1} = \Phi_{\text{diff,cells}}[\{u_i, u_{i+1}\}^k]$$

where

$$\begin{aligned} \Phi_{\text{diff,cells}}[\{u_i, u_{i+1}\}] &= \{u_i + \Delta u, u_{i+1} - \Delta u\} \\ \Delta u &= \frac{1}{2}(u_{i+1} - u_i) \left(1 - \exp \left[-2 \frac{D}{\Delta x^2} \Delta t \right] \right). \end{aligned} \quad (21)$$

The corresponding algorithm is shown in Figure 1. The total rule for diffusion over an entire one-dimensional network of cells is expressed as

$$\begin{aligned} \mathbf{U}^{k+1} &= \Phi_{\text{diff}}[\mathbf{U}^k] \\ \Phi_{\text{diff}}[\mathbf{U}] &= [\text{For } i = 1, 3, 5, \dots; \{u_i, u_{i+1}\} = \Phi_{\text{diff,cells}}[\{u_i, u_{i+1}\}]; \\ &\quad \text{For } i = 2, 4, 6, \dots; \{u_i, u_{i+1}\} = \Phi_{\text{diff,cells}}[\{u_i, u_{i+1}\}]]. \end{aligned} \quad (22)$$

Although the given development is for a one-dimensional line of cells, the concept is readily extended to any multidimensional network of cells.

■ 4.5 Construction of multi-physics transport processes

With rules for elementary processes now available, a complex process consisting of N elementary processes is constructed as a cascade in the form of equation (4). The general transport process, as described in the traditional form by equation (5), can be constructed from some cascading sequence of the elementary processes. One possibility is

$$\mathbf{u}^{k+1} = \Phi_{\text{adv}}[\Phi_{\text{diff}}[\Phi_{\text{react}}[\Phi_{\text{ext}}[\mathbf{u}^k]]]]. \quad (23)$$

The accuracy of this scheme depends on (1) the accuracy of the elementary rules, (2) the accuracy of the splitting and reconstruction process, and (3) the time step. These issues will be addressed in the following section.

5. Case studies

5.1 Individual processes

Before assembling processes consisting of several physical effects, the behavior of the rules developed for the elementary physical processes are examined individually. The external interaction, advection, and reaction kinetics rules given by equations (11), (13), and (16) respectively, are expected to perform well since they come from analytical solutions of the individual rate equations. However, the validity and accuracy of the diffusion rule, as shown schematically in Figure 1 and given by equations (21) and (22), needs to be investigated.

The diffusion rule is examined in Figure 2, where time advances from the top to bottom in the plots. Here we start with a square wave of high-concentration cells in the middle of a network of cells with low concentration. Figure 2 shows the ensuing evolution for various values of the dimensionless diffusion coefficient, $D^+ = D\Delta t/\Delta x^2$. For $D^+ = 0$, the expected exact result of no diffusion is recovered. For relatively low values of D^+ , the predictions match well with those of analytical solutions using Green's functions and traditional finite difference solu-

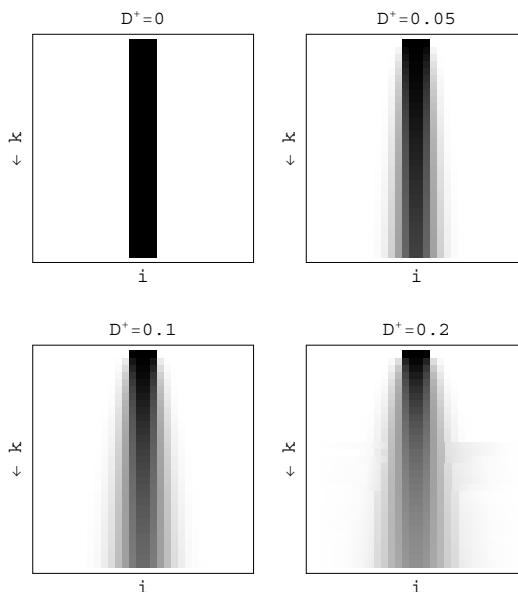


Figure 2. Study of the effect of the dimensionless diffusivity, $D^+ = D\Delta t/\Delta x^2$, on diffusion. Square wave initial distribution is four cells wide. $N_{\text{cells}} = 30$, $k_{\text{max}} = 30$.

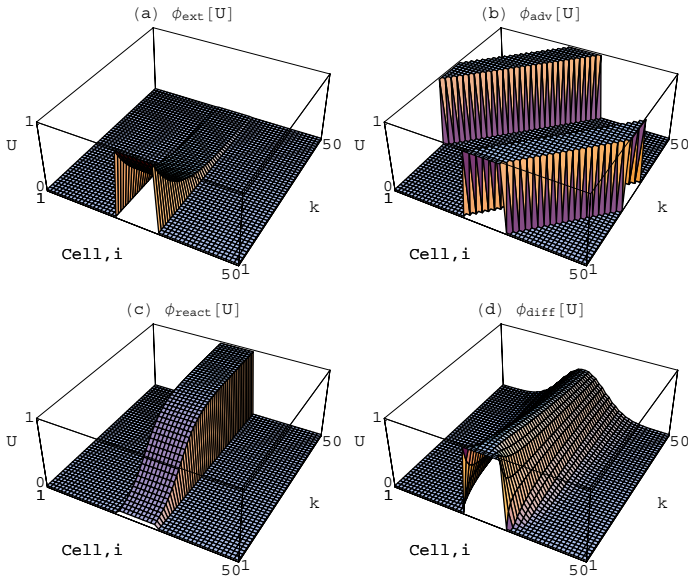


Figure 3. Examination of the elementary transport processes for a square wave initial distribution and wrapped boundaries. (a) External interaction, $H = 0.1$, $g = 0$; (b) Advection, $V = 1$; (c) Logistic reaction kinetics, equation (17), $A = 0.25$, $B = 1$; (d) Diffusion, $D = 0.3$.

tions [1]. However, for relatively high diffusivity, the diffusion effect is repressed since the proposed rules given by equations (21) and (22) can only propagate effects two cells per time level. For the limiting case of $D^+ \rightarrow \infty$ for instance, any initial concentration should instantly spread out evenly over the entire network of cells. It turns out that the results are quite accurate for $D^+ < 1$. A relatively low D^+ can be achieved by using a sufficiently small time step. In general, a small enough time step turns out to be the general criteria for accuracy of the proposed method.

Next the rules for the four elementary transport processes developed in section 4 are examined. Figure 3 shows the response to a square wave initial distribution while Figure 4 shows the same results starting from a random distribution in the cells. Wrapped boundary conditions are used, where the first and last cells are considered to be immediate neighbors. The results fair well compared to expectations. The external interaction mechanism with $g = 0$ produces an exponential decay to the ground state. The advection mechanism translates the initial condition with the specified velocity. Reaction kinetics according to the logistic model give a sigmoidal curve where all initial disturbances approach the stable equilibrium point at $U = B = 1$.

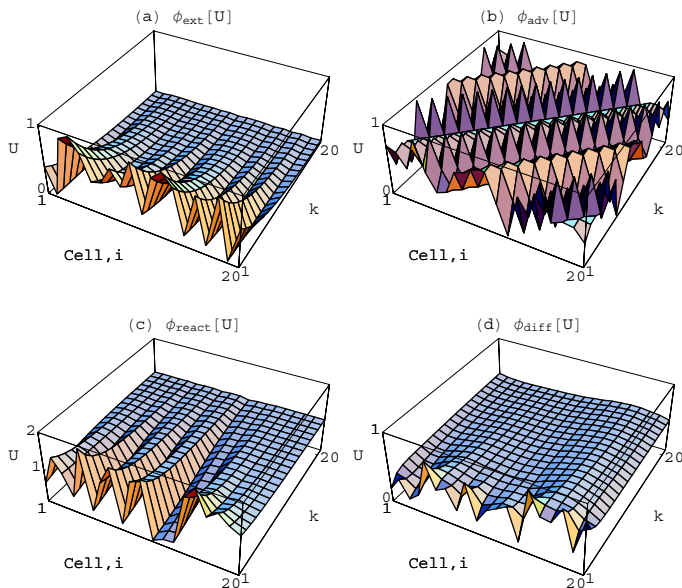


Figure 4. Examination of the elementary transport processes for a random initial distribution and wrapped boundaries. (a) External interaction, $H = 0.1$, $g = 0$; (b) Advection, $V = 1$; (c) Logistic reaction kinetics, equation (17), $A = 0.25$, $B = 1$; (d) Diffusion, $D = 0.3$.

As demonstrated in Figures 2 through 4, each of the rules for the elementary processes gives physically realistic and numerically accurate results when applied individually. In addition, they are simple to program and fast to compute. Next, predictions using multiple processes are examined.

5.2 Multi-physical processes

First a complex process composed of external interaction, diffusion, and advection is examined. The process is constructed with the rule $\phi_{adv}[\phi_{diff}[\phi_{ext}[U]]]$. Results are displayed in Figure 5 for two velocities and two levels of external interaction. The results are not only physically accurate but computationally simple to obtain, since they were computed using a cascade of explicit rules. On the other hand, traditional solutions would require solving the complete transport equation for this process, given by

$$\frac{\partial U}{\partial t} = -V \cdot \nabla U + D \cdot \nabla^2 U - H \cdot U. \quad (24)$$

This equation would take a lot more effort to solve by traditional FD or FE schemes, mainly due to the advection term.

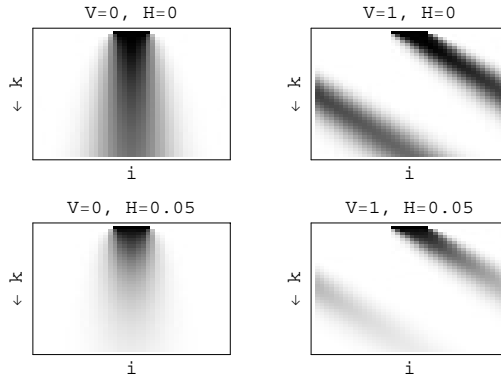


Figure 5. Examination of a multi-physics process consisting of advection, diffusion ($D = 0.25$), and external interaction. Computed using the rule $\phi_{\text{adv}}[\phi_{\text{diff}}[\phi_{\text{ext}}[U]]]$ for a square wave initial distribution and wrapped boundaries.

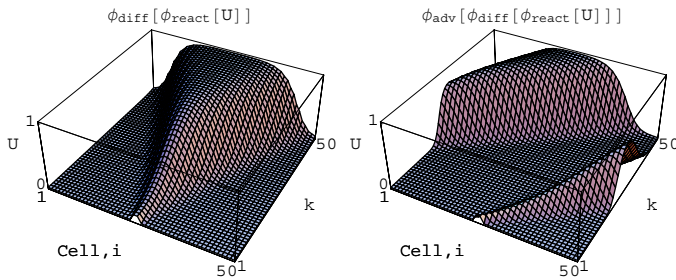


Figure 6. Examination of a multi-physics process consisting of advection, diffusion ($D = 0.25$), and logistic growth kinetics ($A = 0.2$, $B = 1$). Computed using the rule $\phi_{\text{adv}}[\phi_{\text{diff}}[\phi_{\text{react}}[U]]]$ for a square wave initial distribution and wrapped boundaries.

The next example involves reaction kinetics using the logistic growth model of equation (17). Figure 6 shows the application of the rule $\phi_{\text{adv}}[\phi_{\text{diff}}[\phi_{\text{react}}[U]]]$ starting from a square wave initial concentration. The left-hand part of Figure 6 shows a reaction/diffusion process ($V = 0$). As time progresses, a traveling wave is formed; a phenomena only possible in diffusion processes in the presence of nonlinear reaction terms. The right-hand portion of Figure 6 shows the reaction/diffusion process with advection. These particular results are again extremely simple to compute using the current method compared to traditional differential equation methods.

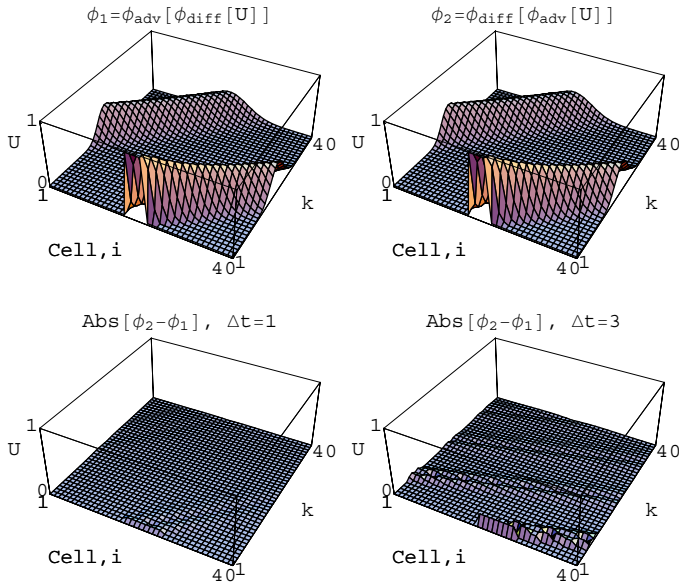


Figure 7. Effect of the order of construction of elementary processes for an advection/diffusion process ($D = 0.25$).

5.3 Accuracy considerations

Although the current method is computationally explicit and simple to implement, an important consideration is the error associated with the order of construction of multi-physics processes. Equation (23) is actually only one of $4! = 24$ possible ways to construct a total process composed of four elementary processes.

An example using the combined advection/diffusion process is demonstrated in Figure 7. Results from applying the rules $\phi_{adv}[\phi_{diff}[U]]$ and $\phi_{diff}[\phi_{adv}[U]]$ are shown along with the difference in the two predictions. Applying the rules in either order produces physically realistic results and relatively small differences between the two predictions.

Numerical experiments reveal that differences caused by the order of construction become increasingly smaller as the time step is decreased. A general observation is that when the time step is small enough such that the elementary rules are accurate, the combined processes exhibit comparable accuracy.

6. Summary and conclusions

A new methodology, based on a combination of cellular automata, traditional finite differencing, and analytical analysis is described. The

method consists of constructing a cascading sequence of simple, explicit rules of evaluation, rather than attempt solutions of complicated partial differential equations. The resulting scheme is computationally explicit yet numerically stable; a combination that does not exist in traditional numerical solutions. In addition to significant modeling flexibility, the cellular automata environment lends itself to extremely efficient computational algorithms and hardware implementation due to its inherent use of local rules and potential for parallel computation.

The power and flexibility of the method is demonstrated by developing solutions for a general transport process. This general transport equation consists of elementary processes due to diffusion, advection, reaction kinetics, and external interaction. Explicit and numerically stable rules for each of these elementary processes are developed. Numerical experiments show that the method is highly accurate if the time step is sufficiently small. The value of the method is that a library of rules for simple, elementary processes can be derived individually. These processes can be assembled in a modular manner in any combination to create models for complex processes.

The modeling and analysis technique presented here is currently being used in a number of applications. One is a study by Vick and Furey [6] of some of the complex thermal/mechanical behavior at sliding contacts in rotating machinery. In general, the method offers a relatively simple means to model complex, multi-physics processes.

Another value of the current methodology is that it frees the user from the shackles of traditional differential equation modeling. One can be imaginative and model observed physical behavior with any suitable set of rules. If the ultimate purpose is to simulate real-world processes, the quality of any proposed cellular automata is ultimately decided by nature itself.

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