Basic Schemes for Reversible Two-Dimensional Cellular Automata

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Two-dimensional reversible cellular automata constructions may have utility for modeling problems that entail inherently reversible processes, such as optical propagation. This paper speculates on the potential of methods articulated in *A New Kind of Science* [1] for addressing inverse problems in optical scatterometry, and then describes preliminary work for two-dimensional reversible cellular automaton schemes.

1. Introduction

1.1 The Model Problem: Statement

This study was first motivated by a conversation with a consultant to the integrated circuit industry. Integrated circuit wafers are optically scanned at several key steps in the production line. If any light-intensity inconsistencies are detected, the line is halted so that a technician may manually inspect the wafer under a scanning tunnelling microscope (STM). "It is too bad you cannot get more information from the optical-array detectors," he said, "because it would really be great to reduce the number, and frequency, of the dreaded trips to the STM."

In this type of optical metrology procedure there are no imaging optics used for the measurements of scattered incident light. Pertinent surface information must be reconstructed solely from optical-intensity measurements in the far-field.

This is an important practical problem because technologies such as nanofabrication and integrated circuit manufacturing utilize optical metrology for noninvasive surface-topography assessments.

1.2 The Model Problem: Why It Is Interesting

The appeal of the problem presented is there are the two fundamental basic science problems conjoined in this otherwise practical application:

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1. electromagnetic scatter from wavelength-scale features, and
2. the inverse problem in optical metrology.

Each of these basic science problems has proved largely intractable with conventional mathematical approaches for reasons we will now consider in turn.

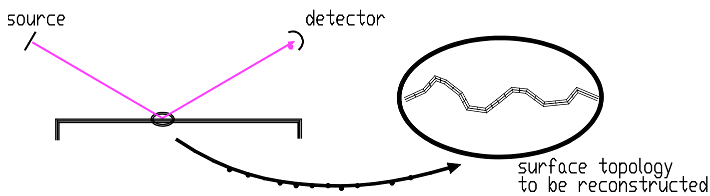

Figure 1. Model problem schematic.

1.2.1 Electromagnetic Scatter from Wavelength-Scale Features

In nanoscale optical metrology, the corresponding direct problem is the capability to predict (far-field) light-intensity measurements (obtained with macroscopic instrumentation) due to electromagnetic scatter from $O(\lambda)$ features. The many orders of magnitude scale variations of this problem preclude conventional direct numerical simulation, even when using sophisticated techniques such as telescoping meshes. Thus, this nanoscale optical scattering problem is an open and quite interesting problem in engineering physics.

1.2.2 Inverse Problem in Optical Metrology

A second computational difficulty of optical metrology is that it is fundamentally an *inverse* problem. Inverse problems arise whenever a system's condition is to be inferred from indirect measurements, and the conventional explanation for their numerical difficulty is that the data is insufficient to uniquely define the state, leading to a formal multiplicity of solutions and the inability to find any solution. Furthermore, lacking a formally complete set of boundary conditions (data), the solution exhibits exaggerated measurement-error sensitivity to whatever data is available.

In describing inverse problem difficulties, most authors focus on the quantification difficulty of the data (e.g., inherent error, insufficient data for a unique solution). Less frequently discussed, but equally important, is the quantification difficulty of the "answer" because, for most inverse problems, the objective is a *qualitative assessment*. Inverse problem data is generally taken to determine the presence or absence of a certain constitutive feature, like "Is there a crack?" or "Is there a pressure spike?" The engineer taking indirect

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measurements knows that there is not enough information to fully characterize the system, and this is not the goal. For example, acoustic measurements on a pipe joint are taken to establish whether or not there is a crack, not to determine the physiognomy of the crack should there be one. However, at present (using, say, a finite element code) one must obtain the *full* unique solution—crack detail, joint geometry, everything—to get *any* solution. Conventional computational methods invariably require full-blown quantitative detail to obtain what is ultimately a qualitative (but often numerically unreachable) answer.

In summary, inverse problems resist numerical solution, even when the underlying science is deterministic, because: (*i*) their data is quantitatively incomplete, and (*ii*) the desired solution is usually a fundamentally qualitative determination.

1.3 The Model Problem: Why Use Two-Dimensional Reversible Cellular Automata?

In this optical metrology application, light is scattered (and measured) principally in a plane. Since the optical metrology model should naturally represent both two-dimensional propagation and irregular boundaries, it seems plausible that two-dimensional cellular automata would offer this capability. Consequently, two-dimensional cellular automata seem the natural choice among the several candidate NKS modeling arrangements. Less evident, perhaps, is the author's conjecture that *reversible* two-dimensional cellular automata evolutions are especially suited to this problem.

While general conceptual frameworks for physical science models in NKS do not yet exist, a possible stratagem is to regard the cellular automata model as if it were an infinitely adjustable analog computer, with fine-tuning imposed through rule specifications. Requiring the cellular automata evolutions to be effectively time-reversible may result in a more natural representation of electromagnetic propagation. (Were one modeling two-dimensional diffusion, for example, reversible cellular automata might not be indicated.)

We now consider the author's preliminary work in two-dimensional reversible cellular automata.

2. Two-Dimensional Reversible Cellular Automata

2.1 Introductory Comments

In cellular automaton methodology, a rule is deemed "reversible" if it is possible to construct an "inverse rule" so that one may compute forward—or backward—from one state to any other state of the system, regardless of the particular configuration. The inherent information conservation [2] of such cellular automaton transformations have

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made reversible rules of particular interest in the modeling of physics [3]. For one-dimensional cellular automata a tiny subset of nearest-neighbor transformation rules can be shown to have inverse rules, and this "reversible-rule" space has received a fair amount of study [4]. However, for two-dimensional cellular automata it turns out that the invertibility of *any* nearest-neighbor transform rule is formally undecidable [5].

Nevertheless, instead of using a single rule, there are alternative composed constructions for reversible cellular automaton algorithms in two dimensions: the second-order Fredkin method, and the Margolus-neighborhood block-transform method. We now consider these formulations in turn.

2.2 Fredkin Second-Order Method

This second-order method for constructing reversible cellular automaton algorithms is attributed to Edward Fredkin [3]. Say that A^-, A, A^+ denote the states of an overall cell assemblage in the prior, current, and next steps, respectively. The conventional means to obtain A^+ from A using rule "ruleX( )" is: $A^+ = \text{ruleX}(A)$. Now, assume that each of the constituent cells in the overall assemblage may assume one of k possible states, numbered $0, 1, \ldots, k-1$. The Fredkin second-order method obtains the next step by

$$A^+ = \text{mod}(\text{ruleX}(A) - A^-,\ k),$$

where mod() denotes the modulus function. To invert the rule, one need only input the states in the reverse sense, that is,

$$A^- = \text{mod}(\text{ruleX}(A) - A^+,\ k).$$

The mod( ) function and requirement that the states be represented as integers are the author's clarification of the original discussion in [3].

The method is second-order because, to generate a state at any given time, one must specify the two preceding states in sequence. This requirement for effectively two initial conditions is typical for models of dynamical systems with inertia. Consequently, evolutions devised using this Fredkin approach would probably be an excellent choice for, say, a simulation of billiard-ball collisions. However, for the envisaged model of light propagation, the author suspects that the two-dimensional reversible cellular automata method described next will prove even more representational.

2.3 Margolus Neighborhood Block-Transform Method

2.3.1 Basic Idea

Block-partitioned strategies [6] (also called the "Margolus neighborhood" in some discussions, e.g., [7]) are not intrinsically invertible *per se*, but can be structured to generate reversible algorithms, as will now be shown. In this method, a block of (say, four) cells is trans-

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formed *as a block* to a new state, again following a lookup table (ruleset) as illustrated in Figure 2.

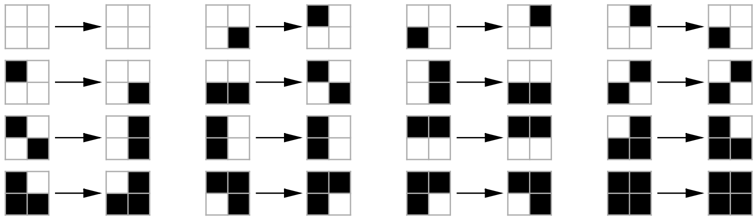

Figure 2. A two-color, reversible, block-transformation ruleset.

The Margolus neighborhood concept works as follows. Contiguous four-cell blocks are defined over the entire two-dimensional cell array. For information to propagate throughout the cell array, the ruleset in each step is applied in two passes. In the first pass, the ruleset is applied on each of the originally-designated four-cell block groupings; in the second pass, the ruleset is applied again on a second set of contiguous four-cell groupings obtained by *shifting* the original block designations *by one cell* in each coordinate direction (see Figure 3).

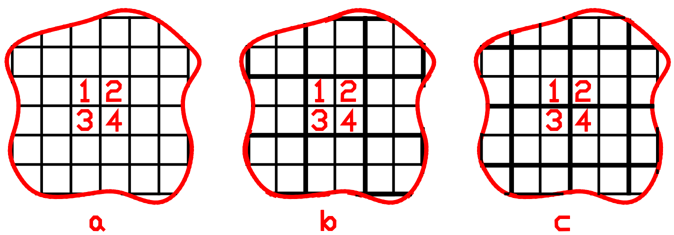

Figure 3. Schematic for block definitions in one (two-pass) step. (a) Cells 1 through 4 identified in a two-dimensional region. (b) Pass 1: transformation ruleset is applied to all 2×2 blocks unshifted; cells 1 through 4 are defined in, and transform within, the same block. (c) Pass 2: transformation ruleset is applied to all 2×2 blocks, shifted; cells 1 through 4 are now each transformed within a different block.

2.3.2 Reversible Block-Transform Rulesets

The specific block-transformation ruleset illustrated in Figure 2 happens also to be invertible, and to obtain the inverse rule one merely reverses the sense of the arrows and resequences the images to facilitate the table-lookup procedure. The ruleset in Figure 2 has two properties which render it reversible.

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1. State (or "color") is conserved: the number of black and/or white cells on either side of each arrow is the same.
2. Every possible configuration (of two-state four-cell blocks) occurs exactly once on the left, and once on the right, side of the arrows.

It turns out that there are 414 720 possible invertible rules for this two-state, four-cell, block-transformation situation.

Figure 4 illustrates a block-transform cellular-array evolution using the invertible ruleset shown in Figure 2. In the first row of Figure 4, the rule is applied for six steps to a 12×12 array of cells (recall that each step involves two applications of the rule); in the second row six steps of Figure 2's *inverse* rule are applied, starting with the last frame of the first row.

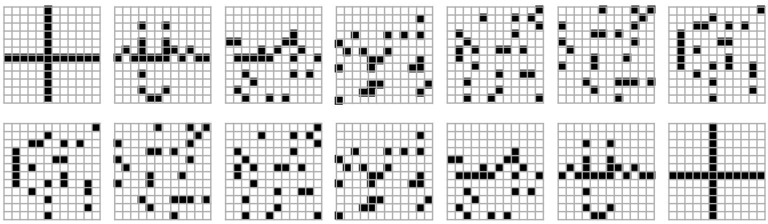

Figure 4. Example of a block-partition reversible-rule evolution. Row 1: The block transformation rule (Figure 2) for six steps. Row 2: The inverse rule for six steps, starting with the last result of Row 1.

The author has devised the capability of enumerating all reversible block-transform rulesets, with the two listed invertibility properties, for an arbitrary number of colors and block sizes. Of course, an inevitable difficulty of cellular automata is that the use of more states (colors) or larger neighborhoods (here, block sizes) leads to an exponential expansion of the rule-space size, as shown in Table 1.

♯ of cells in block	♯ of colors	♯ of block - transform reversible rulesets
4	2	414 720
4	3	7.8393×10^{42}
6	2	2.1567×10^{48}
6	3	9.2328×10^{871}

Table 1. Reversible block-transform rule-space sizes.

2.3.3 Generalized Boundaries using Identity Cell States

The objective of optical metrology is to characterize physical surface (boundary) irregularities. If a cell represents a specific two-dimensional location, then a cell state designated as "boundary" is a logical

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mechanism for defining physical boundaries. Since boundaries are static, a boundary-cell state corresponds to an "identity state"; for example, if the boundary state is red, any cell that is red at the start of the evolution would remain red in every subsequent step. The author accordingly devised the capability of enumerating reversible block-transform rules for arbitrary block sizes, arbitrary number of colors, *and* for an arbitrary subset of those colors designated as "identity states". For example, there are 4 458 052 241 280 block-transformation rulesets possible for the four-cell three-state case, where one of the states is an identity state. (It is still an impossibly large ruleset space, although less than 7.8×10^{42}.)

2.3.4 Isotropic Rules

For modeling optical scatter, a further desirable refinement is a requirement that the propagation phenomena (and, hence, the underlying transformation rules) be independent of the choice of coordinate system, that is, independent of the orientation of the cellular-array definition within the two-dimensional space. The author characterizes this as the "isotropic" requirement on the transformation rulesets. An example of a block-transformation ruleset definition that approximates this behavior, for a four-cell two-state block, is shown in Figure 5.

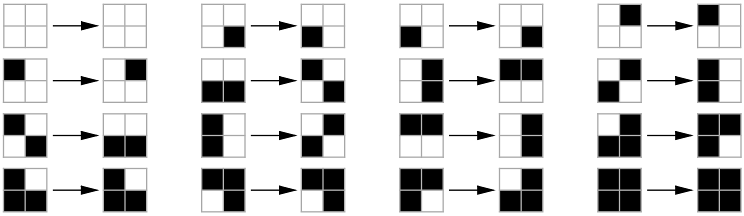

Figure 5. An isotropic block-transform ruleset definition.

The author describes a block-transformation ruleset as "isotropic" if it satisfies the following conditions. Say a and b are two possible con figurations for a block of cells, with configuration b some rearrangement of configuration a. For a block-transformation ruleset to be isotropic, both $a \to b$ and $b \to a$ must be among the ruleset's replacement rules. Restricting the possible transformation rulesets to only those which are isotropic substantially diminishes the rule space. For example, again for the four-cell block situation: with two states modeled there are 7600 isotropic transformation rulesets; with three states, one of these being an identity state, there are 31 876 710 400 isotropic transformation rulesets.

With fewer transformation rules, one might think that isotropic block-transformation rulesets (with possible identity states) would be

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easier to enumerate than the nonisotropic case. Surprisingly, enumerating block-transform rules that are specifically isotropic is a somewhat involved and computationally intensive task that merits a dedicated discussion. So, in lieu of waiting minutes (or longer) for a ruleset list to be generated from a specific rule number, the author has devised schemes that utilize precalculated intermediate results stored on disk to enumerate the rules. About a megabyte of disk space is needed for models utilizing four-cell blocks with three mobile (i.e., nonidentity) states.

In a recent talk [8] the author speculated that (for the purposes of optical metrology) a possibly useful elaboration of the basic Margolus neighborhood scheme may be to discretize the two-dimensional plane into hexagonal assemblages of six triangle cells, rather than the square assemblages of four rectangular cells illustrated in Figure 3. The benefit would be that the fundamentally triangular arrangement might more naturally represent a greater variety of surface topologies, and the hexagonal approach provides two additional natural propagation directions for the scattered quantities. However, the computational requirements of enumerating isotropic rules limits the practical block size to four cells, at least for the preliminary studies.

3. Conclusions

This paper provides some motivation and philosophical background for a recent talk [8] where reversible cellular automata in one and two dimensions were discussed. Two-dimensional demonstrations of the Fredkin approach, of the Margolus neighborhood, and for Fredkin-built-on-top-of-Margolus (block-transform) rulesets, were provided in this talk. The examples collectively illustrated the use of identity colors in reversible algorithms for both conservative and nonconservative evolutions.

This paper has enlarged on the following points relative to this talk.

1. Differential/integral descriptions (and their consequent computational methods) have proved extraordinarily successful for phenomena that can be (meaningfully) quantified.
2. However, many phenomena may resist quantification, and the reasons include: complexity in time and/or space; and/or because their salient descriptive features may be genuinely qualitative.
3. The methodology described in *A New Kind of Science* (NKS) [1] is computationally rich, but also may be a most natural strategy for considering phenomena which resist quantification. This is because the (state) models, data structures, and algorithms of NKS methodology are abstracted idealisms and thus fundamentally qualitative.
4. Optical metrology embodies two fundamental problems, each with quantification ambiguity: (*i*) inverse problems, and (*ii*) the far-field

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measurement of $O(\lambda)$ optical scatter. Consequently, optical metrology might be productively considered using NKS methods.

5. The objective then is to identify candidate NKS algorithms that might naturally represent the physics of two-dimensional optical scatter. Consequently, two-dimensional cellular automaton schemes with properties of:

   - reversibility in time,
   - ability to specify boundaries of arbitrary complexity, and
   - isotropic with regard to the orientation of the cell assemblage,

   have been devised in anticipation of carrying out this research.

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