# Sub-Structuring Lattice Gases*

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**Abstract**

In this paper we apply domain decomposition techniques to lattice gases. We demonstrate how a lattice gas can be modeled by a non-linear partial differential equation using the same classical techniques as were used by Chapman and Enskog in approximating the kinetics of a real gas. As an example, we show how a 1-dimensional viscous Burgers' equation models a specific lattice gas. We then use the domain decomposition ideas for solving this differential equation to develop a sub-structuring technique for this exemplary lattice gas.

## 1 Kinetic Theory of Gases

The kinetic theory of gases was developed to study the non-equilibrium states of gases where they are only slightly removed from equilibrium. Mathematically,properties of the gas are described in terms of a distribution function,$n$. The distribution function, in general, will vary with time and often a non-linear integro- differential equation, viz. Boltzmann's equation, may be derived for the function. As a pertinent example, consider a gas composed of identical molecules of mass $m$. Then, if $n(x,t)$ is the expected number of particles per unit volume at location $x$ at time $t$, Boltzmann's equation is

$$\frac{\partial n}{\partial t} + \xi \cdot \frac{\partial n}{\partial x} = \Delta_{coll} n$$

where $\xi$ is the velocity of each molecule and $\Delta_{coll} n$ represents the changes per unit volume in the number of particles due to collisions, [2].

From mathematical physics it is well known that a valid description of a gas is often given by fluid dynamics. The Navier-Stokes partial differential equations have been applied

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to gas flow problems with remarkable success. Consequently, an often asked question is how well these equations approximate Boltzmann's equation and in turn the kinetics of a gas. An answer to this was provided by the Chapman-Enskog method, [2], which reduces in a constructive manner the kinetic description of a gas in Boltzmann's equation to the fluid dynamics description. Basically, a supposition is made on the distribution function $n$ that it satisfies the regular asymptotic expansion

$$n = \sum_{i=0}^{\infty} \epsilon^i n_i$$

for some small parameter $\epsilon > 0$. The theory then proceeds to show that the Euler equations of hydrodynamics describe the behavior of $n_0$ and the Navier-Stokes equations of hydrodynamics describe the behavior of $n_1$, [2].

In this paper, we will use the ideas of the Chapman-Enskog method to generate a partial differential equation that models the behavior of a given lattice-gas. Moreover, the solution of this equation will have properties that lend themselves to being resolved computationally by domain decomposition techniques. These techniques will be carried over to the lattice gas where a decomposition into sub-lattices will be performed.

## 2 Kinetic Theory of Lattice Gases

According to the molecular theory of matter, a macroscopic volume of gas (say, 1 $cm^3$) is a system of a very large number $M$ of particles moving in a rather irregular way. If the laws of interaction between the particles are perfectly known, the equations describing their motion are

$$\begin{aligned} \frac{d\xi_i}{dt} &= X_i, \\ \frac{dx_i}{dt} &= \xi_i \end{aligned}$$

where $x_i$ is the position vector of the $i$-th particle, $\xi_i$ the velocity vector, and $X_i$ is the force acting upon the $i$-th particle divided by the mass of the particle. In order to compute the time evolution of the system, one would have to solve the $6M$ first-order differential equations. However, solving the above initial value problem for a number of particles of a realistic order of magnitude (say, $M \simeq 10^{20}$) is an impossible and useless task. Consequently, an alternative approach is often taken.

In a lattice gas, the particles are identical with mass $m$ and the irvelocities are restricted to a given set: $\xi_1, \ldots, \xi_p$ with $\|\xi_i\| = \xi, i = 1, \ldots, p$, [4]. That is the velocity vectors have equal modulus, $\xi$,the particle speed. In addition, the particles are confined to move along the edges of a regular lattice. At each node of the lattice, there is a cell associated with it and each cell can be occupied by at most one particle for each allowed velocity. Particles are marched forward in time by successively applying collision and propagation rules. Specifically, to each node $x$ of the lattice and time instance $t$, we attach an occupation number $n_i(x,t)$ to be the number of particles moving in direction $i$. Clearly, by our assumption on the number of particles allowed to occupy a cell, $n_i(x,t) \in \{0,1\}$. If the there are $p$ directions emanating from each node of the lattice, then an occupation vector

| $\alpha$ | | $\beta$ | | $S(\alpha,\beta)$ |
|---|---|---|---|---|
| $\alpha_1$ | $\alpha_2$ | $\beta_1$ | $\beta_2$ | |
| 0 | 0 | 0 | 0 | 1 |
| 0 | 1 | 0 | 1 | $(1+a)/2$ |
| 0 | 1 | 1 | 0 | $(1-a)/2$ |
| 1 | 0 | 0 | 1 | $(1+a)/2$ |
| 1 | 0 | 1 | 0 | $(1-a)/2$ |
| 1 | 1 | 1 | 1 | 1 |

Table 1: Transition Rules ( $0 < a \ll 1$)

$$n(x,t) = \begin{bmatrix} n_1(x,t) \\ \vdots \\ n_p(x,t) \end{bmatrix}$$

is defined. The computation of $n(x,t+\Delta t)$ involves two successive steps: collision followed by propagation. In this situation, collision is the simultaneous application at each node of non-deterministic rules from an in-state $p$-vector $\alpha \in \prod_{i=1}^{p}\{0,1\}$ to be an out-state $p$-vector $\beta \in \prod_{i=1}^{p}\{0,1\}$. Here, $\alpha_i = 1$ indicates an incoming particle in direction $i$ and $\alpha_i = 0$ indicates no incoming particle in direction $i$, and, similarly, $\beta_i = 1$ indicates an outgoing particle in direction $i$ and $\beta_i = 0$ indicates no outgoing particle in direction $i$. Note that $\alpha(x,t) = n(x,t)$. Each transition is assigned a probability $S(\alpha,\beta) = P(\alpha \rightarrow \beta)$ of state $\alpha$ evolving to state $\beta$. The computational advantage of lattice gases is that thecollision and propagation of the particles can be carried out using Boolean logic, [3], implemented either by logical evaluation or table-look-up; it involves no floating point arithmetic.

In this paper, we shall restrict our attention to a one-dimensional lattice gas in which the particles move with velocity $\xi_i = (-1)^{i+1}, i = 1,2$, where $i = 1$ indicates propagation to the right of a node and $i = 2$ indicates propagation to the left of a node. The transition rules are given in Table 1.

Note that

$$n_i(x + \xi_i\Delta x, t + \Delta t) = n_i(x,t) + c_i(n)$$

where $c_i(n)$ is a collision function that can alter the direction of a particle and takes on the values $\pm 1$ or 0. An explicit form of $c_i$ is given by

$$c_i(n) = \sum_{\alpha,\beta}(\beta_i - \alpha_i)S(\alpha,\beta)\ [\ \prod_{j=1}^{2} n_j^{\alpha_j}(1-n_j)^{(1-\alpha_j)}\ ].$$

## 3 Lattice Boltzmann Equation

Having introduced a probabilistic description of the dynamics of a lattice gas, we now turn to mean quantities. In particular, we consider the mean population or ensembled averaged occupation number

$$N_i(x,t) =< n_i(x,t) >$$

where $< \cdot >$ is the average values $n_i(x,t)$ in which $(x,t)$ is fixed. As before, we let

$$N(x,t) = \begin{bmatrix} N_1(x,t) \\ N_2(x,t) \end{bmatrix}$$

be the ensembled occupation vector. Now, if we assume the occupation numbers are uncorrelated then

$$\begin{aligned} C_i(N) &= < c_i(n) > \\ &= \textstyle\sum_{\alpha,\beta}(\beta_i - \alpha_i)S(\alpha,\beta)\ [\ \prod_{j=1}^{2} N_j^{\alpha_j}(1-N_j)^{(1-\alpha_j)}\ ]. \end{aligned} \tag{1}$$

We then get the lattice Boltzmann equation

$$N_i(x + \xi_i \Delta x, t + \Delta t) = N_i(x,t) + C_i(N). \tag{2}$$

With regards to the transition rules given by Table 1, we have

$$C(N) = (C^{(0)}(N) + pC^{(1)}) \begin{bmatrix} +1 \\ -1 \end{bmatrix} \tag{3}$$

where

$$\begin{aligned} C^{(0)}(N) &= \frac{1}{2}(N_2 - N_1), \\ C^{(1)}(N) &= \frac{1}{2}(N_1 + N_2 - 2N_1N_2), \\ p &= \frac{1+a}{2}. \end{aligned}$$

## 4 Chapman-Enskog Expansion

Given the one-dimensional lattice gas whose dynamics are governed by Table 1, we now seek a differential equation whose solution models the gas behavior. To do so, we proceed as in the case of the classical Boltzmann equation described in section 1. That is, we assume a regular asymptotic expansion of $N$,

$$N = \sum_{i=0}^{\infty} \epsilon^i N^{(i)} \tag{4}$$

for some small parameter $\epsilon > 0$. Then,

$$\begin{aligned} N(x \pm \Delta x, t + \Delta t) &= N(t,x) + \frac{\partial N}{\partial t}\Delta t \pm \frac{\partial N}{\partial x}\Delta x + \mathcal{O}(\Delta x^2, \Delta t^2) \\ &= \textstyle\sum_{i=0}^{\infty} \epsilon^i (N^{(i)} + \frac{\partial N^{(i)}}{\partial t}\Delta t \pm \frac{\partial N^{(i)}}{\partial x}\Delta x) \\ &\quad + \mathcal{O}(\Delta t^2, \Delta x^2) \end{aligned} \tag{5}$$

and

$$C(N) = C(\sum_{i=0}^{\infty} \epsilon^i N^{(i)}) = \mathcal{C}(\epsilon) \tag{6}$$

Now,

$$C(\epsilon) = C(0) + \frac{\partial C(0)}{\partial \epsilon}\epsilon + \frac{\partial^2 C(0)}{\partial \epsilon^2}\epsilon^2 + \mathcal{O}(\epsilon^3) \tag{7}$$

Let

$$\begin{aligned} \Delta t &= \epsilon^2 T, \\ \Delta x &= \epsilon L, \\ a &= \epsilon K \end{aligned} \tag{8}$$

for some given constants $T, L, K > 0$. Then on substitution of the expansions (3),(5), and (7) into (2) we obtain

$$C^{(0)}(N^{(0)}) = 0, \tag{9}$$

$$L\frac{\partial N^{(0)}}{\partial x} = \left[\frac{\partial C^{(0)}(N^{(0)})}{\partial N}\right] \cdot N^{(1)} + KC^{(1)}(N^{(0)}), \tag{10}$$

$$T\frac{\partial N}{\partial T} + L^2\left(\frac{1}{2}\frac{\partial^2 N}{\partial x^2} + \frac{\partial^2 N}{\partial x \partial t}\right) = 2\left[\frac{\partial C^{(0)}(N^{(0)})}{\partial N}\right] \cdot N^{(2)} + \left[\frac{\partial^2 C^{(0)}(N^{(0)})}{\partial N^2}\right] \cdot (N^{(1)})^2 + 2K\left[\frac{\partial C^{(1)}(N^{(0)})}{\partial N}\right] \cdot N^{(1)}. \tag{11}$$

Using (3), we see that $C^{(0)}(N^{(0)}) = 0$ implies

$$n_1^{(0)} = n_2^{(0)} \equiv u$$

or

$$N^{(0)} = \begin{bmatrix} u \\ u \end{bmatrix}. \tag{12}$$

Now,

$$\frac{\partial C^{(0)}(N^{(0)})}{\partial N} = \frac{1}{2}\begin{bmatrix} -1 & 1 \\ 1 & -1 \end{bmatrix} \tag{13}$$

is a singular matrix with eigenvalues $\lambda_1 = 0, \lambda_2 = -1$ and corresponding eigenvectors

$$q_1 = \begin{bmatrix} 1 \\ 1 \end{bmatrix}, q_2 = \begin{bmatrix} 1 \\ -1 \end{bmatrix}. \tag{14}$$

Consequently, (11) yields

$$\left[\frac{\partial C^{(0)}(N^{(0)})}{\partial N}\right] \cdot N^{(1)} = L\frac{\partial N^{(0)}}{\partial x} - KC^{(1)}(N^{(0)}) = \left(L\frac{\partial u}{\partial x} - Ku(u-1)\right) q_2.$$

If $N^{(1)} = a^{(1)}q_1 + b^{(1)}q_2$, then it follows that

$$b^{(1)} = L\frac{\partial u}{\partial x} - Ku(u-1). \tag{15}$$

Hence, (11) yields

$$2\left[\frac{\partial C^{(0)}(N^{(0)})}{\partial N}\right] \cdot N^{(2)} = a^{(2)}q_1 + b^{(2)}q_2 \tag{16}$$

where

$$a^{(2)} = -T\frac{\partial u}{\partial t} - L\frac{\partial}{\partial x}\left[Ku(1-u) - L\frac{\partial u}{\partial x}\right] - \frac{L^2}{2}\frac{\partial^2 u}{\partial x^2}$$

Since Range $\left[\frac{\partial C^{(0)}(N^{(0)})}{\partial N}\right]$ = span $[q_2]$, we have $a^{(2)} = 0$. Let $\rho = 2u$, $c = KL/T$, and $\nu = L^2/2T$. Then, $a^{(2)} = 0$ implies

$$\frac{\partial \rho}{\partial t} + c\frac{\partial}{\partial x}(\rho - \frac{1}{2}\rho^2) = \nu\frac{\partial^2 \rho}{\partial x^2}$$

Finally, letting $v = c(\rho - 1)$, we obtain

$$\frac{\partial v}{\partial t} - v\frac{\partial v}{\partial x} = \nu\frac{\partial^2 v}{\partial x^2}, \tag{17}$$

that is, viscous Burgers' equation, [1].

Summarizing, for $\epsilon > 0$, a small parameter, we have that

$$N \simeq N^{(0)} = \begin{bmatrix} u \\ u \end{bmatrix}$$

where $u = \frac{1}{2}(c^{-1}v - 1)$ and $v$ satisfies the Burgers equation (17). Consequently, the behavior of the ensembled occupation vector $N$ can be approximated by the solution of equation (17). Moreover, this equation has been studied extensively and, in particular, the ideas of domain decomposition have bee used effectively to solve it.

## 5 Domain Decomposition

Domain decomposition algorithms for solving equations such as (17) follow a general pattern. First, a numerical time differencing scheme is used to advance the solution over the entire domain. Then, a measurement of the computed solution is taken to determine subdomains of activity. The solution is then recomputed on these sub-domains using a different mesh and possibly a different time differencing scheme. Initial and boundary conditions on the subdomains are obtained by interpolating the data from the computed solution on the global domain,[5].

Since the solution of the equation (17) has been shown to be an accurate approximation of the lattice gas given in Table 1., it seems reasonable to expect that a domain decomposition of the lattice gas using similar ideas as that for Burgers equation would be effective. Specifically, the ensembled occupation vector $N(x, t+\Delta_c t)$ is computed over a coarse lattice and then a first order measurement of its gradient is taken to determine where subdomains of activity are occurring. Initial and boundary conditions on these subdomains are obtained by interpolating the computed values of $N$ on the coarse lattice. The occupation vector is then recomputed on these subdomains using a finer lattice, and the process is repeated at $t + \Delta_c t$.

## 6 Computational Example

We compute the lattice gas given in Table 1 with $a = a_f = 1/8$ and we assume the initial distribution of particles to be given by

$$f(x) = \begin{cases} -\frac{4}{5}x + 1.2, & 0 \le x < .75, \\ \\ -\frac{4}{5}x + 2.0, & .75 \le x \le 1, \end{cases}$$

where $0 \le x \le 1$. That is, for $j = 1, 2$ and $x_i$ an arbitrary node,

$$n_j(x_i) = \begin{cases} 1, & \text{with prob } f(x_i)/2, \\ 0, & \text{with prob } (1 - f(x_i))/2. \end{cases}$$

Particles at the boundary of the global domain are assumed to "wrap around", that is, the boundary conditions are periodic. Nodes on the fine lattice $\mathcal{L}_f$ are separated by a distance of $\Delta x_f = 2^{-11}$ and time steps on $\mathcal{L}_f$ are taken with $\Delta t_f = 2^{-14}$. In this case, we see that Burgers' equation (17) models the gas where

$$\begin{aligned} \nu &= \frac{\Delta x^2}{2\Delta t} = 2^{-9}, \\ c &= \frac{a\Delta x}{\Delta t} = 1. \end{aligned} \tag{18}$$

The quantity $\tilde{u} = (\tilde{v} + 1)$ where $\tilde{v}$ is the computed solution of (17) at $t = 0$, i.e., $\tilde{v}$ is the initial condition, is plotted in Figure 1. There, we see that the subdomain $\tilde{\Omega} = [r, s] = [9/16, 15/16]$ contains the portion of the solution where high resolution is needed. Consequently, we see that the lattice gas with lattice length $\Delta x_f$ need only be implemented in the region $\tilde{\mathcal{L}}_f = \mathcal{L}_f \bigcap \tilde{\Omega}$ and outside of $\mathcal{L}_f$ we can use a coarser lattice $\mathcal{L}_c$. However, changing the lattice mesh length to a larger value can alter the behavior of the lattice gas unless appropriate changes in the bias $a$ is made. Recognizing again that the lattice is approximated by the Burgers' equation (17), we need the lattice gas with lattice mesh length $\Delta x_c > \Delta x_f$ to have as its approximation the same model. Thus, if $\Delta x_c = 2^{-10}$ and $\Delta t_c = 2^{-12}$, then this lattice gas will be approximated by (17) if $a_c = 1/4$. To see this, note that

$$a_f = \frac{\Delta x_f}{2\nu}$$

where $\nu$ is given by (18). Hence a necessary condition for (17) to model the coarse lattice gas is

$$a_c = \frac{\Delta x_f/2}{2\nu} = \frac{1}{2}a_f = \frac{1}{4}.$$

Figure 2 exhibits the ensembled occupation number $\mathcal{N}_c(x, t)$ for $t = .125$ where

$$\mathcal{N}_c(x, t) = N_1(x, t) + N_2(x, t)$$

and $N_1$, $N_2$ are computed from the lattice gas using $a_c$, $\Delta x_c$, and $\Delta t_c$ and superimposed on the finite difference solution of (17). (Here, a first order in time and second order in space

explicit forward Euler method was used to compute the solution of (17).) The ensemble averages in this computation were

$$N_i(x,t) =< n_i(x,t) >= \frac{1}{M}\sum_{i=1}^{M} n_i(x,t)$$

where $M = 2048$ are the number of lattice gases executed and each gas consisted of 1024 cells. Figure 3 illustrates the use of domain decomposition on the lattice gas. Here, boundary conditions on $\tilde{\Omega}$ are furnished by the coarse grid calculation where

$$\begin{aligned} \mathcal{N}_f(r,t) &= N_2(r,t), \\ \mathcal{N}_f(s,t) &= N_1(s,t). \end{aligned}$$

and $N_1$, $N_2$ are coarse grid calculations.

To investigate the effect of the averaging technique on the resolution of the solution, the preceding experiments were repeated using different ensemble averages. In these calculations, spatial averages are also taken, that is, for $i = 1, 2$ we use

$$N_i(x,t) =< n_i(x,t) >= \frac{1}{3M}\sum_{i=1}^{M}(n_i(x-\Delta x,t) + n_i(x,t) + n_i(x+\Delta x,t)).$$

Figures 4 and 5 illustrate the results.

## 7 Conclusions

We have established a relationship between Burgers' equation and a specific lattice gas using Chapman-Enskog techniques as modified in [1]. Using ideas developed in [5] for solving Burgers' equation by domain decomposition, a domain decomposition method was developed for this lattice gas. We furnished computational evidence to support the fact that decomposing lattice gases is possible to achieve the same accuracy with increased performance.

## References

[1] B.Boghosian and D. Levermore , Cellular automoton for Burgers' equation, Complex Systems 1 (1987) p. 17

[2] J. Ferziger and H. Kaper, Mathematical Theory of Transport Processes in Gases, North-Holland Pub., Amsterdam, 1972.

[3] U. Frisch, D. d'Humieres, B. Hasslacher, P. Lallemand, Y. Pomeau, and J. Rivet, Lattice Gas Hydrodynamics in Two and ThreeDimensions, Complex Systems, Vol. 1, No. 4, 1987, pp. 648,707.

[4] R. Gatignol, The hydrodynamical description for a discrete velocity model of gas, Complex Systems, Vol. 1, No. 4, 1987 , pp. 708,725.

[5] A. Perkins and G. Rodrigue, A domain decomposition method for solving the 2-dimensional Burgers' equation, to be published Applied Numerical Mathematics, also available as LLNL report, UCRL - 99823 Rev. 1, Feb. 1989.

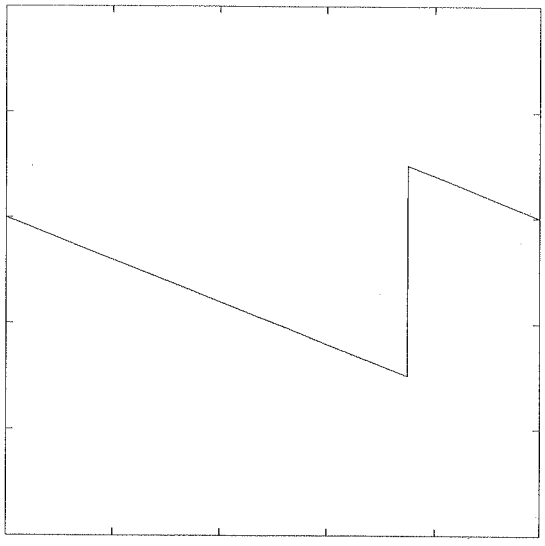

Figure 1: Initial Distribution

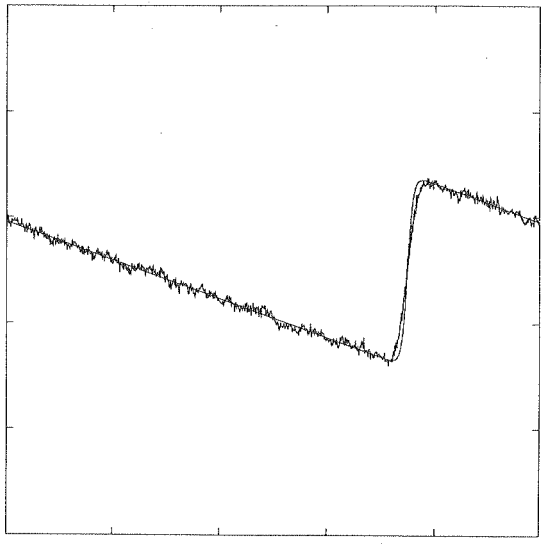

Figure 2: Coarse Lattice Solution Using Only Time Averages

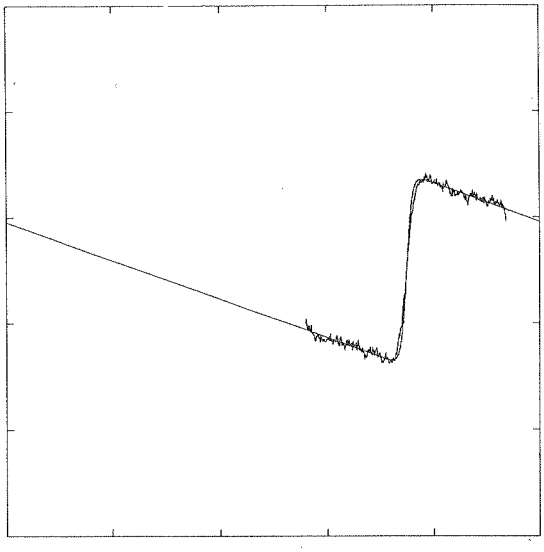

Figure 3: Fine Lattice Solution Using Only Time Averages

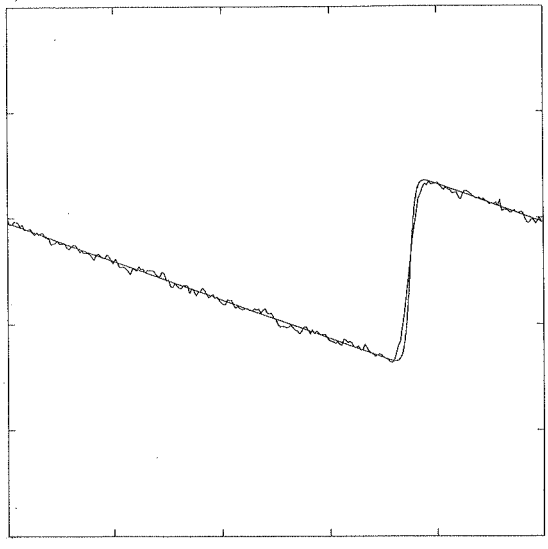

Figure 4: Coarse Lattice Solution Using Time and Space Averages

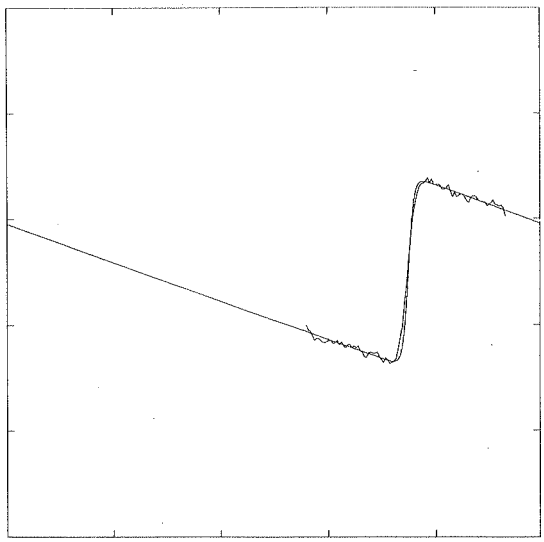

Figure 5: Fine Lattice Solution Using Time and Space Averages