

Two Cellular Automata for Plasma Computations

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Abstract. Plasma applications of computational techniques based on cellular automata are inhibited by the long-range nature of electromagnetic forces. One of the most promising features of cellular automata methods has been the parallelism that becomes possible because of the local nature of the interactions, leading (for example) to the absence of Poisson equations to be solved in fluid simulations. Because it is in the nature of a plasma that volume forces originate with distant charges and currents, finding plasma cellular automata becomes largely a search for tricks to circumvent this nonlocality of the forces. We describe automata for two situations where this appears possible: two-dimensional magnetohydrodynamics (2D MHD) and the one-dimensional electrostatic Vlasov-Poisson system. Insufficient computational experience has accumulated for either system to argue that it is a serious alternative to existing methods.

1. Two-dimensional magnetohydrodynamics (2D MHD)

The basic equations of two-dimensional incompressible magnetohydrodynamics are a relatively straightforward generalization of those of two-dimensional fluid mechanics, and for our purposes can be written as [1-3]:

$$\frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla p + \mathbf{j} \times \mathbf{B} + \rho \nu \nabla^2 \mathbf{u}, \quad (1.1)$$

$$\frac{\partial}{\partial t}(\rho A_z) + \nabla \cdot (\rho \mathbf{u} A_z) = \rho \eta \nabla^2 A_z, \quad (1.2)$$

$$\nabla \cdot \mathbf{u} = 0. \quad (1.3)$$

Here, $\mathbf{u} = (u_x, u_y, 0)$ is the velocity field and $\mathbf{B} = (B_x, B_y, 0)$ is the magnetic field. The mass density, assumed uniform and constant, is ρ , and the pressure is p . For all variables, $\partial/\partial z = 0$. The magnetic field \mathbf{B} is obtained from a one-component magnetic vector potential $\mathbf{A} = (0, 0, A_z)$ as $\mathbf{B} = \nabla \times \mathbf{A}$. The electric current density is $\mathbf{j} = \nabla \times \mathbf{B} = (0, 0, -\nabla^2 A_z)$ in this geometry. The pressure p is obtained from solving the Poisson equation that results from taking the divergence of equation (1.1) and using $\nabla \cdot \partial(\rho \mathbf{u})/\partial t = \rho \partial(\nabla \cdot \mathbf{u})/\partial t = 0$.

The dissipation coefficients ν and η are the kinematic viscosity and magnetic diffusivity respectively. In the natural dimensionless units of the problem, they may be thought of as the reciprocals of either (a) the Reynolds number ($\nu \rightarrow R^{-1}$) and magnetic Reynolds number ($\eta \rightarrow R_m^{-1}$) or (b) the Lundquist number ($\eta \rightarrow S^{-1}$) and the "viscous" Lundquist number ($\nu \rightarrow M^{-1}$). The choice (a) is preferable when comparable magnetic and fluid kinetic energies are expected, and the choice (b) when the fluid kinetic energy is expected to be small or zero. Idiomatically, these are the "astrophysical" and "controlled fusion" regimes, respectively.

The generalization of fluid-dynamic cellular automata methods to equations (1.1) through (1.3) present essentially two challenges, over and above those associated with two-dimensional Navier-Stokes fluids. First, equation (1.1) differs from the two-dimensional Navier-Stokes equation only by the presence of the extra volume force $\mathbf{j} \times \mathbf{B}$ on the right-hand side. For the two-dimensional geometry, $\mathbf{j} \times \mathbf{B} = -(\nabla A_z) \nabla^2 A_z$, so all magnetic quantities are determined *locally* by A_z . Given A_z , the inclusion of $\mathbf{j} \times \mathbf{B}$ presents neither more nor fewer significant complications than the inclusion of external forces such as gravity now present in operating two-dimensional Navier-Stokes codes; this will be discussed presently.

The second new feature is the advancement of A_z , and it can be dealt with by a straightforward extension of methods introduced for the hexagonal lattice gas model [4-7]. The cells and molecules are identical to those of the hexagonal lattice gas, but in addition, each molecule carries with it a "photon label," or quantum of A_z , associated with an index $\sigma = +1, -1$, or 0. Each molecule can execute the same two-dimensional, momentum-conserving, Fermi-Dirac collisions that it executes in fluid simulations, carrying its value of σ with it. Each hexagon now contains eighteen possible single-particle states instead of six. A particle's σ can change only in collisions for which $\Sigma \sigma = 0$. The field A_z is interpreted as an average of σ over super-cells containing many adjacent hexagons, in the same way that the fluid velocity \mathbf{u} is interpreted as the average of the particle velocity $\hat{\mathbf{e}}_a$ ($a = 1, 2, \dots, 6$) over super-cells containing many adjacent hexagons.

It appears to be possible and desirable to restrict the σ -exchanging collisions to those two-body collisions for which the initial pairs of σ -values are $(+1, -1)$, $(-1, +1)$, and $(0, 0)$. For each of these three initial possibilities, it is convenient to choose as the outcome one of the same three possible pairs of values, randomly, with each one of the three possibilities as equally likely (probability 1/3). In hexagons with two or more particles per $\hat{\mathbf{e}}_a$, no colli-

sion occurs—the final state is the same as the initial one. Though it is not an essential feature of the physics, the σ variable may be thought of as the z -component of canonical momentum for fluid particles bearing (both signs of) charge for motions confined to a plane. However, the particle motions underlying the true microphysics are far more complicated than this argument would indicate, and they are many approximations removed from 2D MHD. Their inclusion, in a way that reflected the microphysics as faithfully as the mechanical scattering rules represent the molecular collisions, would require particles of two mass species, z -velocities, z -accelerations, and so on.

The inclusion of the $\mathbf{j} \times \mathbf{B} = -(\nabla A_z) \nabla^2 A_z$ force in equation (1.1) apparently cannot be dealt with within the pure cellular automaton framework without the necessity of replacing the configuration-space cells by phase space cells (see section 2). In this respect, it is apparently a matter similar to the inclusion of gravity in the two-dimensional Navier-Stokes case and can be dealt with in the same way that gravity is now included in the Los Alamos code. Define $\langle A_z \rangle$ as the macroscopic average of σ over, say, $(64)^2$ hexagons. $\nabla \langle A_z \rangle$ and $\nabla^2 \langle A_z \rangle$ can then be obtained from local finite-difference approximations. Inside each super-cell, hexagons may be chosen randomly in proportion to the components of $-(\nabla \langle A_z \rangle) \nabla^2 \langle A_z \rangle$, and particles are flipped to admissible unoccupied values of \hat{e}_a to provide the requisite momentum per unit time per unit volume, as indicated by $-(\nabla \langle A_z \rangle) \nabla^2 \langle A_z \rangle$.

A Chapman-Enskog development can be given for any model kinetic equation which contains a collision term which conserves x and y momenta in particle collisions, conserves $\Sigma_\sigma \sigma$, and obeys an H-theorem [5,8–10]. The Fermi-Dirac statistics require an eighteen-valued distribution function f_a^σ at each hexagon. For theoretical purposes, f_a^σ can be interpreted as a smooth, spatially-differentiable ensemble average. The mass, momentum, and vector potential densities, also assumed smooth, are defined by $\rho = \Sigma_{a,\sigma} f_a^\sigma$, $\rho \mathbf{u} = \Sigma_{a,\sigma} \hat{e}_a f_a^\sigma$, and $\rho A_z = \Sigma_{a,\sigma} \sigma f_a^\sigma (\cos(2\pi a/6), \sin(2\pi a/6))$, $a = 1, 2, \dots, 6$, and $\sigma = 1, -1, 0$.

The differential conservation laws are:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \quad (1.4)$$

$$\frac{\partial}{\partial t}(\rho \mathbf{u}) + \nabla \cdot \Pi = 0 \quad (1.5)$$

$$\frac{\partial(\rho A_z)}{\partial t} + \nabla \cdot \phi = 0 \quad (1.6)$$

where $\Pi \equiv \Sigma_{a,\sigma} \hat{e}_a \hat{e}_a f_a^\sigma$ and $\phi = \Sigma_{a,b} \hat{e}_a \sigma f_a^\sigma$. Π and ϕ are the momentum flux tensor and vector potential flux vector respectively.

The local thermodynamic equilibrium distribution is [10]

$$f_a^\sigma(eq.) = [1 + \exp(\alpha + \beta \mathbf{u} \cdot \hat{e}_a + \gamma \sigma A_z)]^{-1} \quad (1.7)$$

where the Lagrange multipliers α , β , γ are obtained from requiring that equation (1.7) lead to ρ , \mathbf{u} , and A_z . Explicit calculation of α , β , γ requires that, as in the Navier-Stokes case, we assume $u^2 \ll 1$ (small Mach numbers). Solving for α , β , γ , $f_a^\sigma(\text{eq.})$ becomes, up to terms of $O(u^3)$,

$$\begin{aligned} f_a^\sigma(\text{eq.}) = & (\rho/18) \left\{ 1 + 2\hat{e}_a \cdot \mathbf{u} + 3\sigma A_z/2 \right. \\ & + \left(\frac{9-\rho}{18-\rho} \right) [2(2\hat{e}_a\hat{e}_a : \mathbf{u}\mathbf{u} - u^2) \\ & \left. + \frac{3}{2} \left(\frac{3\sigma^2 A_z^2}{2} - A_z^2 \right) + 6\sigma\hat{e}_a \cdot \mathbf{u}A_z] \right\} \end{aligned} \quad (1.8)$$

Inserting $f_a^\sigma(\text{eq.})$ in equations (1.4) through (1.6) gives the Euler equations:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \quad (1.9)$$

$$\frac{\partial}{\partial t}(\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u}\mathbf{u}) = -\nabla \cdot \mathbf{P} \quad (1.10)$$

$$\frac{\partial}{\partial t}(\rho A_z) + \nabla \cdot \left[\rho \mathbf{u} \frac{2(9-\rho)A_z}{(18-\rho)} \right] = 0. \quad (1.11)$$

In equation (1.10), \mathbf{P} is the pressure tensor is

$$\mathbf{P} = (\rho/2) \left[1 - \left(\frac{9-\rho}{18-\rho} \right) u^2 \right] \mathbf{1} - \left(\frac{9}{18-\rho} \right) \rho \mathbf{u}\mathbf{u}. \quad (1.12)$$

At low densities ($\rho \ll 9$), the combination $2(9-\rho)/(18-\rho) \rightarrow 1$ so that equation (1.11) becomes the nondissipative version of equation (1.2), and $\mathbf{P} \rightarrow (\rho/2)(1 - u^2/2)\mathbf{1} - \rho \mathbf{u}\mathbf{u}/2$ as in the fluid case [4,5,7].

The imperfections in the model are two-fold: the \mathbf{u} -dependent \mathbf{P} , which has the same form in the Navier-Stokes case, and the absence of the $\mathbf{j} \times \mathbf{B}$ term on the right-hand side of equation (1.10), which, as already discussed, involves going outside the model. (At this level, the transport of A_z is still that of a "passive scalar.")

The Chapman-Enskog procedure [10] may be carried to first order in the ratio of mean-free path to macroscopic length scale, and leads to ($u^2 \ll 1, n \ll 9$):

$$\left(\frac{\partial}{\partial t} + \hat{e}_z \cdot \nabla \right) f_a^\sigma(\text{eq.}) = \left(\frac{2\hat{e}_a\hat{e}_a - \mathbf{1}}{18} \right) : \rho \nabla \mathbf{u} + \frac{\sigma \hat{e}_a}{12} \cdot \rho \nabla A_z = \Omega_{a,\sigma}^{(1)}(f) \quad (1.13)$$

The right-hand side of equation (1.13) stands for the linearized (about $f_a^\sigma(eq.)$) collision term which might contain, say, the 2R, 2L, and 3S collisions (Wolfram's notation [5]) appropriately generalized for the σ -exchange.

$\Omega_{a,\sigma}^{(1)}(f)$ is, in general, an 18×18 matrix acting on an 18-component column vector $f_{a,\sigma}^{(1)}$, and is difficult to invert, even without allowing for other potential complications such as finite lattice size effects [11]. The solution for $f_{a,\sigma}^{(1)}$ has not been carried out, but from the form of the middle part of equation (1.13), it will be seen to contain terms involving $\rho \nabla u$ and $\rho \nabla A_z$. These, in turn, seem certain to lead to terms in equations (1.5) and (1.6) proportional to $\nabla \cdot (\rho \nabla u)$ and $\nabla \cdot (\rho \nabla A_z)$ respectively. In the incompressible limit, these are the standard viscous and resistive dissipative terms of equations (1.1) and (1.2). The coefficients ν and η have been calculated by Hatori and Montgomery [15].

The inclusion of "stopped" particles will make these coefficients even more difficult to calculate, and as in the case of real substances, "measurement" may provide more reliable values than theoretical calculation.

2. One-dimensional Vlasov cellular automata

The one-dimensional, electrostatic, Vlasov-Poisson system advances particle distribution functions $f_j(x, v, t)$ and an electric field $E(x, t)$, which accelerates particles in the x direction. In the continuous two-dimensional phase space (x, v) , f_j obeys

$$\frac{Df_j}{Dt} \equiv \frac{\partial f_j}{\partial t} + v \frac{\partial f_j}{\partial x} + \frac{e_j E}{m_j} \frac{\partial f_j}{\partial v} = 0 \quad (2.1)$$

in dimensionless units [12]. The symbol f_j represents two different distributions: $j \rightarrow i$ for positive ions and $j \rightarrow e$ for electrons. For the electrons, $e_e = -1$, and for the ions, $e_i = +1$. For the electrons, $M_e = 1$, and for the ions, $M_i = M$, an arbitrary integer > 1 . (The cellular automaton is designed to eliminate all floating-point operations.) The velocity space is infinite, $-\infty < v < \infty$, and a variety of boundary conditions may be assumed in x . For present purposes, we will assume ideal reflecting plates at $x = 0$ and $x = L$, no external electric fields, and zero net charge between $x = 0$ and $x = L$. This results in $f_j(0, v, t) = f_j(0, -v, t)$, $f_j(L, v, t) = f_j(L, -v, t)$, $E(0, t) = E(L, t) = 0$, and can be implemented by choosing periodic initial conditions of period $2L$ subject to the initial symmetry $f_j(x, -v, 0) = f_j(-x, v, 0)$, which will be preserved in time. L is a (large) integer.

The electric field $E(x, t)$ obeys Poisson's equation

$$\frac{\partial E}{\partial x} = \int_{-\infty}^{\infty} (f_i - f_e) dv \quad (2.2)$$

and in one dimension may be obtained from Gauss's law [13,14]. For the present assumptions about the boundary conditions, it may be written as

$$E(x, t) = \int_0^x dx' \int_{-\infty}^{\infty} dv (f_i(x', v, t) - f_e(x', v, t)) \quad (2.3)$$

in $0 < x < L$.

In the cellular automaton version, the phase space is divided into square cells of integer dimension for both species, so that $x \rightarrow n$, $n = 1, 2, 3, \dots, L$; $v \rightarrow s$, $s = -\infty, \dots, -1, 0, 1, \dots, \infty$, although in practice, all v -cells above some large but finite $|s|$ will always be empty. Time is discretized into integer steps $\tau = 0, 1, 2, 3, \dots$. Inside each phase space cell, the discretized distribution functions $f_j(n, s, \tau)$ are always either 1 or 0. Fermi-Dirac statistics are assumed, as initial conditions, and are preserved by the automaton now to be described. The discretized electric field is $E(n, \tau)$, which will also be an integer.

The updating of the $f_j(n, s, \tau)$ and $E(n, \tau)$ takes place in three steps. At $\tau = 1, 4, 7, \dots$, $f_j(n, s, \tau)$ is updated in the x direction according to

$$\begin{aligned} f_j(n, s, \tau) &= f_j(n - s, s, \tau - 1), \\ (\tau &= 1, 4, 7, \dots). \end{aligned} \quad (2.4)$$

At $\tau = 2, 5, 8, \dots$, $f_j(n, s, \tau)$ is updated in the v direction according to

$$\begin{aligned} f_i(n, s, \tau) &= f_i(n, s - E(n, \tau - 1), \tau - 1), \\ f_e(n, s, \tau) &= f_e(n, s + ME(n, \tau - 1), \tau - 1), \\ (\tau &= 2, 5, 8, \dots). \end{aligned} \quad (2.5)$$

(Equations (2.5) and (2.6) reflect the accelerations of ion and electrons.) Finally, at $\tau = 0, 3, 6, 9, \dots$, the electric field is updated according to the discretized version of Gauss's law which is

$$\begin{aligned} E(n, \tau) &= \sum_{n'=0}^n \sum_{s=-\infty}^{\infty} [f_i(n', s, \tau - 1) - f_e(n', s, \tau - 1)], \\ (\tau &= 0, 3, 6, 9, \dots) \end{aligned} \quad (2.6)$$

Equation (2.7) is not a local determination of $E(n, \tau)$ and cannot be made so. It can, however, be updated in a somewhat more local way. Namely, establish $E(n, 0)$ by equation (2.7), then determine $E(n, \tau)$ for $\tau \geq 3$ by counting the net numbers of charges which pass into or out of the region between $x = 0$ and $x = n$ by counting those which go past the n^{th} cell in both directions. Since equation (2.7) simply gives $E(n, \tau)$ as the total number of positive charges minus the total number of negative charges which lie between the first and n^{th} cells, this number, once established, can be updated by the local operation of counting flow past a point (this is the discretized version of the one-dimensional Maxwell equation $\partial E / \partial t + 4\pi j = 0$).

At this point, so little analysis of the automaton given by equations (2.4) through (2.7) has been done that it is pointless to speculate about how effective a competitor it can be made to established methods of solving the one-dimensional Vlasov equation such as particle-in-cell or Fourier-Hermite spectral techniques. Some points clearly need to be analyzed, such as the manifest nonconservation of energy associated with updating the electric field at different time steps from those at which the velocity space is updated (equations (2.4) to (2.7), though the net nonconservation of energy over a three-unit cycle τ may be quite small). That the recipe is in some sense a convergent algorithm for the Vlasov equations seems almost obvious, with the convergence enhanced by spreading the velocity-space distribution, for a given number of particles per fixed phase-space volume, over more and more cells in s . That no floating-point operations are involved is also manifest. There is nothing sacred about the order in which the three steps (2.5), (2.6), and (2.7) are carried out, and it may be determined in practice that another order is superior.

Equations (2.4) through (2.7) are perhaps the first example of a *phase-space* cellular automaton, as contrasted with a *configuration-space* one. It seems inevitable, in circumstances where in nature the system is such that local fluid variables do not suffice to determine the distribution function, that phase space considerations must arise. The Vlasov equation is perhaps the first and simplest example. Once again, however, a local conservation law has played a crucial role: equation (2.1) is a statement of the local conservation of f_j itself [14].

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References

- [1] D. Fyfe, D. Montgomery, and G. Joyce, *J. Plasma Phys.*, **17** (1977) 369.
- [2] A. Pouquet, *J. Fluid Mech.*, **88** (1978) 1.
- [3] S. A. Orszag and C. M. Tang, *J. Fluid Mech.*, **90** (1979) 129.
- [4] U. Frisch, B. Hasslacher, and Y. Pomeau, *Phys. Rev. Lett.*, **56** (1986) 1505.
- [5] S. Wolfram, *J. Stat. Phys.*, **45** (1986) 471.
- [6] D. d'Humières, Y. Pomeau, and P. Lallemand, *C.R. Acad. Sci. Paris, Ser. II*, **301** (1985) 1391.
- [7] J. P. Rivet and U. Frisch, *C.R. Acad. Sci. Paris, Ser. II*, **302** (1986) 267.
- [8] R. Gatignol, "Théorie Cinétique des Gaz à Répartition Discrète des Vitesses", *Lecture Notes in Physics*, **36** (Springer-Verlag, Berlin, 1975).

- [9] J. H. Ferziger and H. G. Kaper, *Mathematical Theory of Transport Processes in Gases* (North-Holland, Amsterdam, 1972).
- [10] D. Montgomery and G. D. Doolen, *Physics Letters A*, **120** (1986) 229.
- [11] B. Boghosian and D. Levermore, "A Cellular Automaton for the Burgers' Equation", *Complex Systems*, **1** (1987) 31.
- [12] B. Adler, S. Fernbach, and M. Rotenberg, eds. *Methods in Computational Physics, 9: Plasma Physics* (Academic Press, New York, 1970).
- [13] J. M. Dawson, "The Electrostatic Sheet Model for a Plasma and its Modification to Finite-Size Particles", in *Methods in Computational Physics*, B. Adler, S. Fernbach, and M. Rotenberg, eds. (Academic Press, New York, 1970) 1-28.
- [14] D. C. dePackh, *J. Electron Contr.*, **10**, (1962) 13a. See also: K. Symon, D. Marshall, and K. W. Li, in *Proc. 4th Conf. on Numerical Simulation of Plasmas*, J. P. Boris and R. A. Shanny, eds. (Washington, D.C.: Office of Naval Res., 1971) 68-125.
- [15] T. Hatori and D. Montgomery, "Transport Coefficients for Magnetohydrodynamic Cellular Automata", *Complex Systems*, **1** (1987) 734.